What makes a material function?

Let me compute the ways…

Modelling in FP7 NMP Programme

Materials projects

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Edited by

Lula Rosso and Anne F de Baas

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CONTENT

3.3 Micromagnetism

(length-scale 1 nm - 100 mm time-scale 1ps-1000ns, sometimes even atomic)

Chapter 4 Continuum modelling of materials

4.1 Continuum mechanics

4.1.1 Solid Mechanics

4.1.2 Fluid Mechanics

4.1.3 Continuum Thermodynamics

4.2 Chemistry

4.3 Electromagnetism (optics, magnetics, electrical)

Chapter 5 Process and device modelling

Chapter 6 Linking of models and numerics

6.1 Linking of models

6.1.1 Linking between different electronic models

6.1.2 Linking between electronic and atomistic models

6.1.3 Linking between electronic and continuum models

6.1.4 Linking between different atomistic models

6.1.5 Linking between atomistic and mesocale models

6.1.6 Linking between mesoscale and continuum mechanics

6.1.7 Linking between atomistic and continuum mechanics

6.1.8 Linking between different continuum models

6.1.9 Combination of flow models with thermomechanics

6.2 Numerics

6.2.1 Accelerated simulations models

6.2.2 Post processing

Chapter 7 Development of models

7.1 Modelling of fundamental equations

7.2 Modelling of constitutive equations

Chapter 8 Applications of models

Chapter 9 Modelling in Industry

Chapter 10 Achievements of the models beyond experiments

Annexes

Annex 1 FP7 NMP Projects fiches

Annex 2 List of existing simulation software

Introduction

Modelling is a powerful tool that supports materials research in the development of novel or improved applications. It provides the key information for identifying new materials, tailoring materials and design materials for structures and systems.
To foster dialogue and mutual understanding between industrial end-users, software developers and theoreticians, this publication presents the scope and achievements of the modeling in about 50 projects funded in the 7th Framework Programme (2007-2013) by the NMP Programme, unit Materials.

Importance of the projects to the European Industry

The use of materials modeling in industries is very versatile. Application addresses fields like Energy, Environment, Transport, Health, ICT and Manufacturing. It is supporting the creation of products like solar cells, sensors, car parts, tissues, computers, tools, coatings. Industrial application is the target of the FP7 NMP program and the projects show the continuous effort to move from model development to model application and finally upscaling for industrial application. It is important to note that, in general, models become most useful to industry when they have reached an advanced maturity. This requires strong interaction between the code developers and industry, and, because of the complexity and long timescale of the code development and validation process, the support of programmes such as NMP makes an important contribution to competitiveness.

The most crucial issue related to modeling in industrial applications is in the formulation of models that produce realistic results. In general, modeling and simulations can be the eyes of the experimentalists, helping them to access information that would not be available otherwise and interpret the experimental results. Modeling provides also invaluable predictions on the evolution of a system in a quicker or cheaper way than with trial and error methods. Industry uses modelling for:

- Saving costs by establishing a strategy for testing and by screening new material candidates, when a “try and fail” approach cannot be carried out in the industry or it would be too complicated, dangerous or expensive.
- Understanding results of measurements. This is particularly important at the nanoscale and at femtoscale where access to materials properties and processing methods is often difficult. The simulation can provide this information for every point in the sample at every time.
- Reducing the time to market, by accelerating the time scales of understanding and developing new materials.
- Suggesting new materials and experimental procedures to create them. Materials design by modeling is about investigation of relations between chemical and physical composition, microstructure and effective properties at a macroscale, so that a material can be designed with desired macro-properties. Modeling can be used to examine the properties of materials and devices that have not or cannot yet be created.

Questions that can be answered by modelling

To show the value of modeling, the achievements of the models beyond experiments have been listed. The models can answer questions like:

•What is the influence of the automotive catalytic converter's shape on its performance?
•Which hydrogen-microstructure interactions play a critical role in the degradation of materials and components?
•Which are the dissipation mechanisms that contribute to the macroscopic adhesion between a metal and a polymer?
•What is the role of thermodynamics and what are the reversal processes involved in ultrafast magnetisation processes?
• Is it possible to control the parameters of the excitation process and of the metal oxides to create long-lived metastable phases with tailored physical properties?
• Which is the role of the size of the systems in realistic nanometric devices? How is the dynamics influenced when the length scale is reduced to the nanometer size of devices (<20 nm)?
•Which are the parameters that control the final state in a solar cell reached after the photo-excitation?
• Which is the influence of biomedical devices on the surrounding tissues?
• What is the most adequate stiffness and permeability of an intervertebral disc substitute?
• Which is the increase of electrical conductivity in composites upon addition of carbon nanotubes?

What are models? What are simulations?

Materials are complex systems and the equations that describe the physical and chemical behaviour of real systems are often too complicated to be solved easily. In order to save computer time, which is a precious and limited resource, the description of phenomena has to be simplified. Fortunately, often not all details need be taken into account in order to reproduce and predict experimental results. Key assumptions about reality can be made ignoring the complexity that is not necessary to describe the given situation. In this brochure, these approximations are called "models"[1].

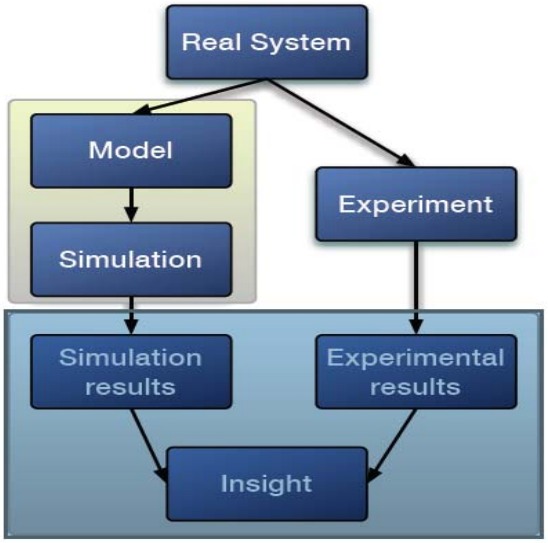

Fig 1 Simulation gives the numerical solution to the model applied to a specific situation (Hans Fangohr, University of Southampton, UK)

With "simulation software and numerics" it is meant instead the implementation of the model in a computational code and the numerical methods that are used to solve the equations. In this publication, modelling is considered to be the establishing of relations between physical or chemical quantities.The tuning of constants in an existing relation (parameterisations like force fields or engineering rules) are not considered to be modelling.

[1] *Note: the word "model" is used in many other situations (e.g. geometrical model of the sample, car model or fashion model), but different words will be used here for those instances.*

Model application and model development

Application of models

A model is strong if it is transferable from one materials system to another within the limits of the model. Many NMP projects are applying existing physics and chemistry models to new materials and manufacturing processes. This has generated a wealth of new information[2]. When applying an existing model to a new situation, unexpected results or new phenomena may be discovered, but these results are obtained with existing equations. An overview of the extensive fields of model application in FP7 NMP projects will be described in Chapter 8 in more detail.

Development of new models

At times, models cannot be transferred from one physical situation to another (say from energy conversion to spin-dynamics). In such cases, research projects may want to increase the complexity of the model, by incorporating new physics and chemistry. This happens when complete new physics and chemistry is to be described. Modellers start from the simpler equations, and gradually add complexity to it (e.g. more transition metal orbitals, ligand orbitals, Coulomb exchange, spin-orbit, phonons) until a satisfactory agreement with experiments is reached. For example, it has been necessary to develop new models in femtosecond dynamics: at the femto-scale new dynamics, physics or chemistry takes place and new opto-electronics/magnetics/bio/chemistry models have been developed. Alternatively, modelers apply the model first at a small scale and transfer the results into a larger scale model in the form of constitutive equations. Constitutive equations are necessary to close the equations describing the system. Together they form the governing equations. This allows them to identify what are the critical relevant processes that lead to experimental results. Another typical case of the necessity to develop new models are the constitutive equations for continuum processes at the macro-scale. Existing macro-scale models consider processes at a smaller scale approximately and thus, by their nature, do not incorporate all necessary physics/chemistry. This often happens in mechanical modeling e.g. when considering how to build a structural model of an amorphous material in some smart way.

Chapter 7 will briefly describe the situations in which new physics and/or chemistry equations have been developed. In this chapter, adhering to the above definition of the word "model", only new equations are discussed. For example, the fine tuning of an existing force field to better reproduce results of a new material but using the same established equations is not considered as a new model in this text but as a new application of the same model. On the other hand, developing a new force field by adding new terms to include physical or chemical properties previously excluded will be considered as a new model.
New constitutive equations linking physical or chemical parameters in a new empirical equation, found as results of modeling or as results of experiments, are also included as new modeling. The basic phenomenon might not be completely understood but this new relation can at least be called an 'hypothesis' .

Text in the fiches describing developments of models and constitutive equations are highlighted in yellow.

[2] *Please note that the physical/chemical knowledge about the system or process needed to perform the model application goes beyond purely computational skills.*

Intermezzo: Some philosophy

The conservation equations are the foundations of physics and chemistry. Modeling starts with an approximation which at first is seen as a good balance between complexity and computability. Development of models may either make the crude model more complex (and in principle the perfect conservation equations is retrieved) or reduce the complexity of the model.
Below (Fig. 2), is an illustration of model development, across time and length scales.

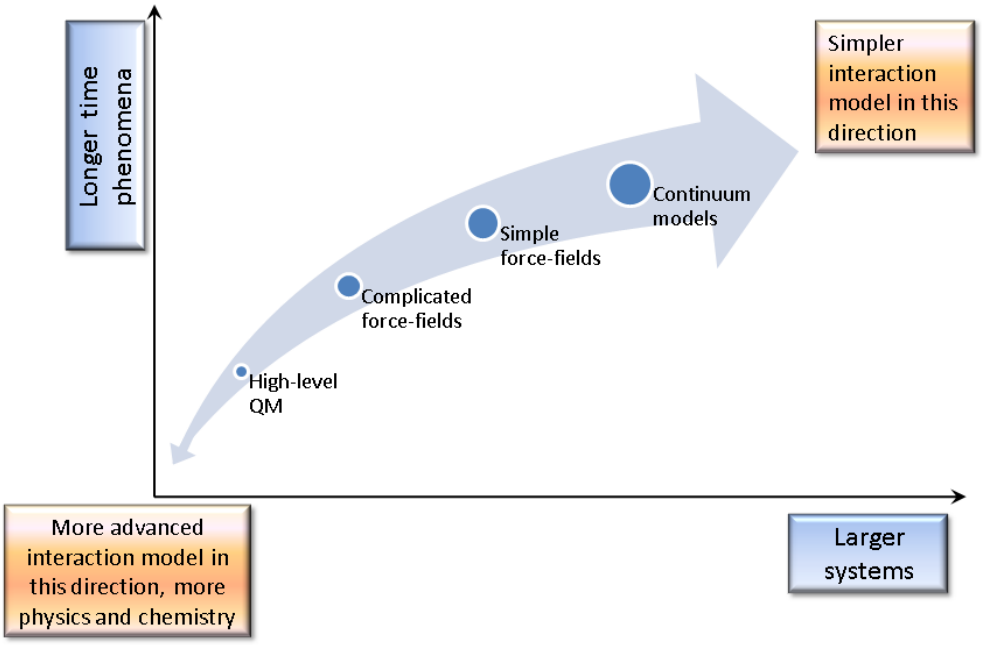

Fig 2 Model development works by moving along the arrow upwards or downward. (Kersti Hermansson, Uppsala University, SE)

Method development

The word "method" is reserved to indicate the way in which models are used. For example, the development of a smart way to compute long-range interactions in materials quickly and accurately is considered here method development rather than model development (although at the same time it certainly allows the use of more advanced interaction models because the simulation goes faster).

Other examples of method development are the methods to improve the sampling of complex potential energy landscape and phase space; this is called metadynamics. Since it can be particularly difficult to sample efficiently the phase space of a material for realistic conditions, improvements on current methods are valuable for the materials community, see Chapter 2 and 6.2 for more information.

Choosing the right model

When several (validated) models exist, the scientist/industry has to choose which one to use. This "testing of models" is also a valuable part of modelling. This consists in trying to answer questions like "which model gives properties that are closest to measurements for this material?" Here the researcher is investigating which physics is needed to describe the given situation. So a model that “approximate reality by considering the neighbours as point charges and ignore temperature effects” states what is the necessary physics to describe the measurements with. Sometimes the choice of a model depends on the balance

between accuracy and simplicity. The outcomes of such testing might also be important because if none of the models are adequate the result of testing is that more physics/chemistry needs to be added to existing models.

MONAMI has been testing two models to calculate the electronic structure of V_2O_3: a so called N-th order Muffin-Tin Orbital (NMTO) model, with features like massive down folding and generation of Wannier combined, and full-potential software using dynamical mean field theory for strongly correlated systems.

In MORDRED, large-scale atomistic simulations of oxide interfaces using dynamic charge transfer models were benchmarked against first principles simulations. Calculations of structure and charge for a large set of cluster, bulk and interface cases with both models were compared to undertands the limits of the faster and more approximated method.

OXIDES has been doing comparative tests of two first-principles methodologies, PSIC and B1-WC, by applying them to structural, electronic, and magnetic properties of a known 2-dimensional electron gas system: LaAlO3/SrTiO3. They evaluated the reliability of PSIC and B1-WC, comparing them with theoretical results presented in literature or obtained with other methods. This way, they explored the limits and capabilities of the two approaches. This testing is essential in selecting the most adequate band energy description to be exploited for transport properties, but it is not stricto sensu a new model development.

Numerical power needed and up-scaling for the industry

Simulation of models applied to new materials involves finding a solution to the equations of the model. This can become very complicated and the computational power needed may become an issue.
Design environments should be developed that balance accuracy and speed. To this end, many models are solved with parallel algorithms, which allow the load to be distributed among computer processors.
Upscaling to industry should build on the progress made in High Performance Computing (HPC), theoretical models and faster numerical processes.
Part of the effort should be directed towards the key and transverse issues of software code modularity and reusability. An integrated and user-friendly design environment must be created. This might require vertically integrated communities with theoretical modelers, experimental data generation and validation experts, software and hardware integrators and industry end-users.

Introduction of model types

Types of models

A convenient way of approaching materials modeling consists in separating the models according to the physics or chemistry involved. This is often related to the time and length scale of the processes and determines the size of the systems that can be simulated with certain available computer resources. For example, modeling of chemical reaction at the nanoscale, and ion transport thereafter.
The four natural levels usually addressed are:

Method	**Number of atoms**	**Length scale**	**Time scale**
Electronic models	10-100	0.1-1 nm	-
Atomistic models	10^2-10^9	0.1-100 nm	fs -μ s
Mesoscale models	10^6-unlimited	100 nm - mm	ms -s
Mesoscale magnetism models		1 nm - 100 mm	1 ps – 1000 ns
Continuum approaches	Unlimited	mm	ks

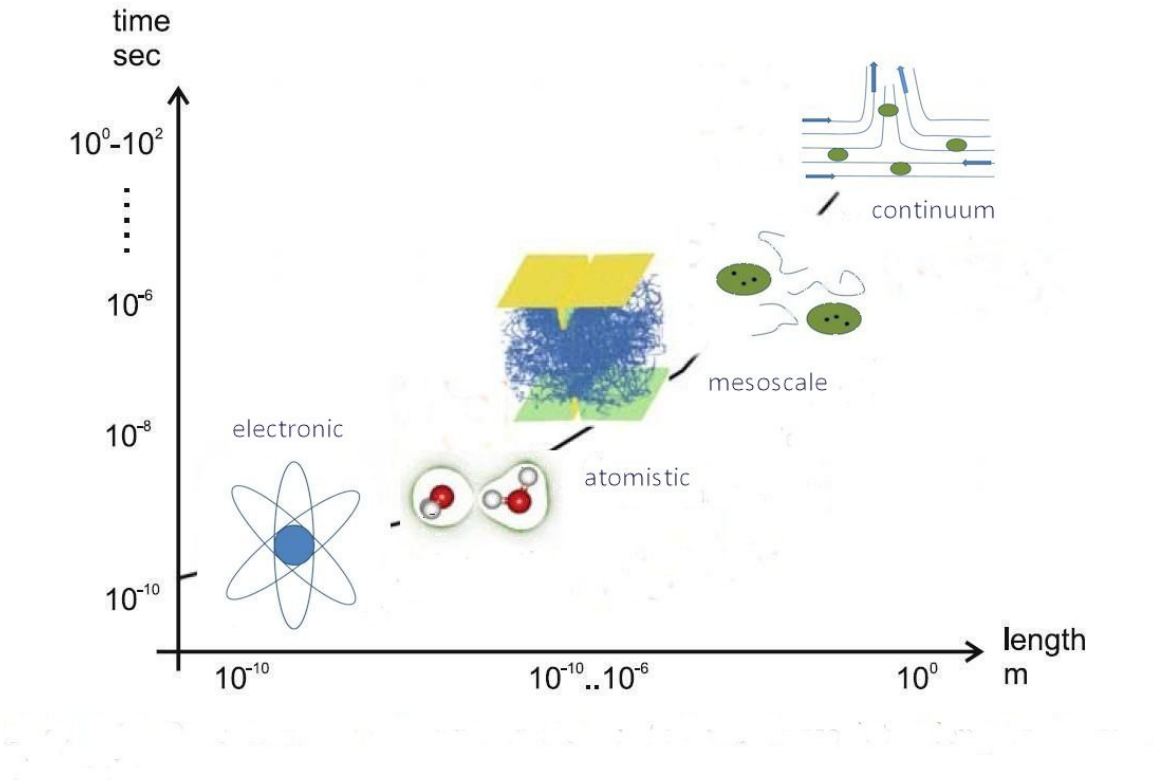

Fig 3 An illustration of models valid at their typical length and time scales (Pierre Severin, Coexpair and Olaf van der Sluis, Philips)

Electronic scale: Ab initio models calculate electronic structures "from first principles" (i.e. based on fundamental principles of physics) expressed in the Schrödinger's equation within a set of approximations that do not include fitting the model to experimental data. These models thus rely on basic and established laws of nature without ad hoc parameterisation. Here, the material is explicitly represented by nuclei and electrons. Quantum mechanical methods are used to describe the behavior of the electrons which determine the properties and structures of the material. From the model results at these shortest atomic time/length scales, electronic transitions and chemical reactions can be derived.

> *Examples of electronic model results:*
> *Electronic band structure giving conductive/dielectric and optical properties*
> *Thermodynamic stability and kinetic elementary processes for atomic defects and dopants*

Atomistic scale: In addition to quantum mechanics based techniques, atomistic modeling establishes effective interactions between atoms, called interatomic potentials (also empirical potentials or force fields). Interatomic potentials do not treat the quantum nature of electrons explicitly, which allows models using these potentials to be enormously faster than models using quantum methods. Such interatomic potential based modeling may not be as accurate as full quantum mechanical approaches but can be used to simulate complex materials processes as radiation damage in nanocrystalline materials and friction between surfaces.
When the electronic degrees of freedom are ignored, molecular mechanical models and classical mechanics are applied to describe the behavior of atoms and molecules. The most common technique here is Molecular Dynamics simulations, now routinely carried out on systems including up to tens of thousands of molecules (consisting of many atoms) over tens of nano seconds. At these longer time scales e.g. lattice motion, electronic transport are described.

> *Examples of atomic model results:*
> *Diffusion parameters, surface and interface energies.*

Mesoscopic scale: At the supra-atomic scale where uninteresting or fast details of the atomic motions are averaged out or replaced by stochastic terms, mesoscopic models concentrate on essential motions and large-scale structures. Examples are the so-called coarse-grained models in which the fundamental unit is a "bead" that interacts with other "beads" via effective soft potentials. This scale also includes macro-spin approaches that combine atomic spins into a macro-spin.

> *Examples of mesoscopic model results:*
> *Morphology of thin oxide films deposited with plasma processes*
> *Spin waves spectra in spintronic devices*

Macroscopic scale: At this level material is assumed to be continuously distributed throughout its volume. Models at this scale disregard the discrete particle-based structures and smaller detail. This is how materials are seen and touched. Modelling at this scale can predict material decomposition, defect formation, crack propagation, solidification of liquids and other important variables for industrial manufacturing. At these macroscopic length scales e.g. thin films and realistic nano-devices with metallic contacts are described.

Examples for macroscopic model results:
Flux of ink in an ink-jet process
Conductance of a contacting finger in an electronic device
Load transfer in a biomedical device

In the next chapter, the models in each category will be introduced and it will be described how they are used in FP7 NMP materials projects.

Linking of models (multi-scaling and multi-physics/chemistry modeling)

In order to increase their predictive capability and applicability to a wide range of applications, macro-scale models need to include processes, which originate at the nano- and micro-scale. This lies in the very nature of the macro-scale models, where atomistic effects are neglected. For example, macro-scale models that approximate interfaces by a set of effective band offset parameters have no predictive power over interface related effects as the detailed atomistic and electronic structure near the interfaces is not taken into account while it determines the annihilation of excited atoms.

The great challenge in creating accurate and predictive models is that materials form a true multi-scale problem. A consistent hierarchy of simulations at different levels of representation is needed to generate results at the molecular level that can be used at a larger scale level. Multi-scaling is connecting different codes, each dealing with part of the physics/chemistry at a different scale with a different level of detail and complexity. Multi-physics/chemistry modeling is connecting different codes describing different physics/chemistry at the same scale.

A major issue in linking models is the reduction, extraction and transfer of data from one model to another and this is a very active subject of research. For example, semi-empirical pseudo-potentials, which can be used to calculate the accurate electronic structure, are based on first principles calculations at a smaller scale (Hartree-Fock, density functional theory, and higher level QM methods). In continuum modeling often the results of models applied at meso-scale (nm) are fed into the macro-scale model (μm) in the form of constitutive equations or as boundary conditions and represents a big challenge in contemporary modeling.

Finally, last but not least, in a multi-scale multi-physics approach not only models should be connected but also integrate experimental data in a clever way.

Modelling for interpretation of experimental results/characterization

The interpretation of experimental data as material properties relies on models as well. In Fig 1 "experimental results" contains BOTH the "getting the signal" phase and "making the interpretation" phase. This includes deciding which formula (model) to use to convert the signal into a property. It can also involve the post-processing of measured quantities into other physical/chemistry properties.

METACHEM is processing transmission, reflection and ellipsometry spectra of metamaterials measured at different angles of incidence (ellipsometric data) to extract values of optical constants of metamaterial. This is done with the help of electromagnetic wave propagation models, but the interpretation model used is at the moment a debated research topic discussing the existence of concepts like "refractive index".

Chapter 1
Electronic models

The theoretical framework of electronic models is the Schrödinger equation, which provides a description at the quantum level of any atomic or molecular system evolving with time. All electrons are considered explicitly.

The most general form of the Schödinger equation is

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

where i is the imaginary unit, ħ is the reduced Planck constant, Ψ is the wavefunction of the quantum system, which depends on time and on the positions, momenta and spins of all particles in the system. Often the spin part of the wavefunction is not explicitly carried in calculations that do not focus on magnetic properties. This convention is followed below. The most crucial element is H, the Hamiltonian operator, which represents the total energy of any given wavefunction and takes different forms depending on the external forces acting on the material. In magnetics, the Hamiltonian includes terms expressing energy due to exchange interaction, spin-orbit interaction, and Zeeman interaction.

In practice, quantum mechanical models are finding suitable approximations of the full Hamiltonian and/or of the molecular orbitals, in order to simplify the numerical calculations without compromising the quality of the simulated results.

1.1. Ab initio quantum mechanical (or first principle) models

The Schrödinger equation can be solved exactly only for a few problems of very limited interest. To solve the equation for systems of practical use, approximations are in general required. *Ab initio* models may be based on a series of approximations that do not include fitting the model to experiments. This is also called a first principle approach because the model is using the Schrödinger equation and is still based purely on fundamental principles of physics.

Quantum mechanical chemistry models are routinely used to calculate the ground state of atomic and molecular systems and the energy and configurations (electronic structure) of the excited states. This can be applied to several problems of practical use.

Ab initio models are applied, to calculate the mechanism of new catalysts and proton conductance in proton exchange membranes (HYPOMAP) surface energies and activation energies of catalytic nanoparticles (NEXT-GEN-CAT).

Interface processes can also be studies at the quantum level, for example adhesion of metal-ceramic interfaces and internal grain boundaries in realistic conditions (ROLICER) ;

interfacial hydrogen bonding and adsorption of water and carbohydrates on cellulose surfaces (SURFUNCELL); the energy barriers and binding energies of hydrogen in normal interstitial sites and around point defects (MULTIHY);

In solar cell material development, ab initio models are used to calculate changes in the work functions of metal electrodes upon deposition of self-assembled monolayers (MINOTOR) and to calculate the formation energy of inclusion complexes in layered magnesium oxides, HTLC, which is relevant for the synthesis of quasi-solid electrolytes, and the energy, electronic distribution and properties of nanostructures in PV excitonic solar cells (INNOVASOL). These models can also cover superconducting systems and are then used to predict electronic and superconducting properties at interfaces of layers with different axis orientation (SUPER-ION).

Given the challenges of solving the Schrödinger's equation, quantum mechanical calculations can only be performed for isolated systems (in vacuo) and at zero temperature. However, often the output of ab initio quantum mechanical models is used as input to develop parameters for models at higher scales, in the development of interatomic potentials or to calculate partial atomic charge distribution. This ensures the incorporation of crucial quantum effects and properties for larger, more realistic, systems simulations at a reduced computational costs and time.

The Schrödinger equation can be solved for small molecular systems exactly if one considers that the mass of the nuclei is much larger than the mass of the electrons, the Born-Oppenheimer approximation. This assumption is valid if the electrons move much faster than the nuclei and the electrons feel the electric field of the nuclei *as if* the nuclei are in a fixed position. The electronic wavefunction of the electrons depends then only on the position of the nuclei and not on their momenta.

Basis sets

To solve the Schrödinger's equation numerically the concept of basis sets of wavefunctions is introduced. The molecular orbitals are expanded as a linear combination of such functions with the weights or coefficients to be determined.

Often a simple and effective basis set is made of linear combinations of atomic orbitals (LCAO) centered in the nuclei. Basis set composed of Gaussian functions centered on the nuclei are also popular because of their flexibility in implementation and, only if needed, functions centered on bonds or lone pairs are added.

In solids and other systems with periodic boundary conditions, it is more appropriate to use basis sets composed of plane waves up to a cutoff wavelength. These functions are naturally periodic and independent of the atom positions and are therefore appropriate to describe the delocalized electrons in solid crystal (electron gas).

In all cases, the choice of the most appropriate basis functions depends on the system under consideration and the level of accuracy that is needed in the final result. A large number of ready-made basis sets are available and implemented in commercial codes, but new basis set are sometimes generated to study systems that present new challenges.

Electronic structure calculations are usually performed with a minimal basis set, e.g. the minimal number of functions that are required to represent all the filled orbitals in each atom. However, it may be necessary to refine (at the cost of computational speed) the minimal basis set with functions that are able to contribute to specific geometric and nuclear effects, like polarisability functions to treat more accurately electron distribution asymmetry. Also diffuse functions may be added for calculations of the electronic excited-state, electric field property, and long-range interactions, such as Van der Waals forces, and, last but not least, for systems in which a considerable portion of the electron density is far away from the nuclei.

1.1.2 Hartree-Fock (HF) method

The Hartree–Fock (HF) method is often the starting point of molecular poly-electron structure calculations. The molecular orbital is represented as the sum of single electron atomic orbitals each multiplied by a corresponding coefficient. The coefficients of the expansion are obtained numerically using a variational procedure that iteratively refines the individual electronic solutions to obtain the configuration that yields the lowest total energy (also known as SCF, self-consistent field).

Several approximations are applied. First, the Born-Oppenheimer approximation is assumed and relativistic effects are neglected. Moreover, each particle is thought to be subjected to the mean field created by all other particles. This means that the method is neglecting the electron-electron correlation terms in the Hamiltonian. This method thus fails to represent strongly correlated systems, and systems close to the dissociation limit.

1.1.3 Higher level ab initio methods

The Hartree-Fock method has two fundamental limitations. Firstly, the molecular orbitals are represented as linear combination of single electron orbitals. This provides a localised representation of molecular orbitals which is not appropriate in highly dispersive systems. Secondly, electron correlation is neglected. Higher level quantum chemical methods have been developed to overcome these simplifications and provide the most accurate calculation results of electronic structure.

These methods include: Configuration Interaction (CI), which includes the excited states in the description of the electronic state. Coupled Cluster (CC) takes the basic Hartree–Fock molecular orbital method and constructs multi-electron wavefunctions using the exponential cluster operator to account for electron correlation. Møller–Plesset perturbation theory (MP2, MP3, MP4, etc.) improves on the Hartree–Fock method by adding electron correlation effects as a second order perturbation of the Hartree-Fock Hamiltonian. These methods devise schemes which can, at least in principle, be infinitely refined by the addition of higher level terms. For example, a CCSD(T) calculation simply means a calculation done using a coupled-cluster method, which includes singles and doubles fully and triples are calculated non-iteratively.

Note that due to their higher computational cost, these methods can only be applied to systems very limited in size.

1.1.4 Density Functional Theory[1]

A popular and versatile quantum mechanical method that includes the effect of electron correlation (albeit approximately) is Density Functional Theory (DFT).

DFT is based on the Kohn-Hohnberg theorem that states that ground-state energy is uniquely defined by the electron density. The properties of a many-electron system are then determined by using functionals, i.e. functions of the spatially dependent electron density. DFT calculations usually consist in solving the Kohn–Sham equation which is the Schrödinger equation of a fictitious system (the "Kohn–Sham system") of non-interacting particles (typically electrons) that generate the same density that the real system of interacting particles would generate. This simplifies the formulation greatly because instead of explicitly including the real potential of many interaction electrons, the Kohn–Sham equation contains a local effective (fictitious) external potential of non-interacting particles.

Typically, the biggest additional modeling necessary in DFT is the formulation of the exchange-correlation functionals, which need to model not only the electron exchange and correlation energy terms but also the difference between the kinetic energy of the fictitious non-interacting system and the real one. The equations are then solved using an iterative self-consistent approach based on the variational principle.

The simplest way to implement DFT is using the local density approximation (LDA) where the functional depends only on the density at the coordinate where the functional is evaluated. A further refinement is obtained considering the generalized gradient approximation (GGA) which is still local but also takes into account the gradient of the density at the same coordinate.

In solid state calculations, the local density approximations are still commonly used along with plane wave basis sets, consistent with an electron gas approach, which is appropriate for electrons de-localised through an infinite solid. In molecular calculations, however, more sophisticated functionals are needed, and a huge variety of exchange-correlation functionals have been developed for chemical applications. Among physicists, probably the most widely used functional is the revised Perdew–Burke–Ernzerhof exchange model (a direct generalized-gradient parametrisation of the free electron gas with no free parameters); however, this is not sufficiently calorimetrically accurate for gas-phase molecular calculations. In the chemistry community, one popular functional is known as BLYP (from the name Becke for the exchange part and Lee, Yang and Parr for the correlation part). Even more widely used is B3LYP which is a hybrid functional in which the exchange energy, in this case from Becke's exchange functional, is combined with the exact energy from Hartree–Fock theory. Along with the component exchange and correlation functionals, three parameters define the hybrid functional, specifying how much of the exact exchange is mixed in. The adjustable parameters in hybrid functionals are generally fitted to a 'training set' of molecules. Although the results obtained with these functionals are usually sufficiently accurate for most applications, unfortunately, there is no systematic way of improving them (in contrast to some of the higher level ab initio methods like

[1] *Large parts of this paragraph have been taken from Wikipedia.*

configuration interaction or coupled cluster theory). In the current DFT approach, error is estimated comparing the results to other methods or experiments.

In many cases the results of DFT calculations for solid-state systems agree quite satisfactorily with experimental data. Computational costs are relatively low when compared to traditional methods, such as Hartree–Fock theory and higher level ab initio methods based on the complex many-electron wavefunction. Despite recent improvements, there are still difficulties in using density functional theory to properly describe intermolecular interactions, especially van der Waals forces (dispersion); charge transfer excitations; transition states, global potential energy surfaces and strongly correlated systems; and there are inaccuracies in DFT calculations of the band gap in semiconductors. Its incomplete treatment of dispersion can adversely affect the accuracy of DFT (at least when used alone and uncorrected) in the treatment of systems which are dominated by dispersion (e.g. interacting noble gas atoms) or where dispersion competes significantly with other effects in biomolecules. Improving DFT calculations by modifying the functional or by the addition of terms to overcome this problem is an active research topic.

Spin polarized DFT is an extension of DFT which includes both the electron density and the up and down spin densities explicitly in the Kohn-Sham equations. This is used to calculate to calculate the magneto-crystalline anisotropy and the exchange interaction between atomic spins (ULTRAMAGNETRON, REFREEPERMAG, MAGNONICS, DYNAMAG, ATHENA, CRONOS).

1.2. Many body models and effective Hamiltonians

A large class of many-electrons systems can be studied theoretically by the models that have been discussed in the previous paragraph. In fact, their electronic bands are typically well reproduced by DFT. However, when the system size increases, the calculations required by full ab initio methods become very quickly unfeasible. In addition, ab initio methods are commonly solved through approximations which limit their accuracy. For example, in highly correlated systems and in solids where electrons may be considered as nearly localised, solving the Schrödinger equation within an independent electron scheme fails to reproduce experimental results.

Many-body models are commonly used in solid state physic, to calculate band structure and properties like electrical resistivity and optical absorption. Also the phenomena at metal-insulator interface can be described (LEMSUPER).

Except in few simple cases, models that treat many-body electron interactions require the definition of an "effective" Hamiltonian. This is a simplified representation of the true Hamiltonian where some parameters are derived from empirical data. These methods are very popular because they allow to treat large systems (up to millions of non-equivalent atoms), where a full ab-initio method without the approximations would be computationally too expensive.

A similar problem is encountered when it is necessary to include the effect of the surroundings on the system of interest. Models are developed that provide a simplified way to describe these interactions considering the background medium as a continuum. An example is solvation models where the weak interactions with the solvent molecules are treated approximately to keep the computational costs limited.

1.2.1 Nearly-free electron model

The electronic band structure of metals can be described by the simplest effective Hamiltonian, which treats electrons in a solid as moving almost freely through the crystal lattice.

1.2.2 Many body approaches

The many body Dynamical Mean Field Theory (DMFT) is a method designed to deal with strongly correlated materials. In such materials, the approximation of independent electrons, which is used in Density Functional Theory band structure calculations, breaks down. DMFT includes the local interactions between electrons and bridges the gap between the nearly-free electron gas model and dense condensed-matter models.

> *One of DMFT's main successes is the description of the phase transition between a metal and a Mott insulator a process where the strength of electronic correlations increases. DMFT has been successfully applied to real materials to calculate material properties of strongly correlated systems like high temperature superconductors (MONAMI, GOFAST, LEMSUPER).*

Quantum Monte Carlo provides a direct representation of the many-body wave function, which is unfortunately accompanied by of statistical uncertainty. However this can be reduced by longer simulation times. For example, the Hartree-Fock approximation can be used as starting point of the many-body wavefunction and then be multiplied by any symmetric function designed to represent the correlations. Monte Carlo methods are used to solve efficiently the equations which are typified by very large sparse matrices.

> *Quantum Monte Carlo methods have been used to derive a DFT exchange-correlation functional which was used in molecular dynamics to calculate adsorption of light-weight hydrogen (HYPOMAP) and calculate thermodynamic properties of single and double perovskites many body Hamilton problem at finite-temperature problem (ATHENA)*

Alternatively, pseudopotentials can be developed that approximate the motion of the core (i.e. non-valence) electrons of an atom and its nucleus with an effective potential, or pseudopotential. Thich approach considers the nuclear charge as effectively screened by tightly bound core electrons. As a consequence, only the chemically active valence electrons are treated quantum mechanically, thereby reducing the number of electrons in the Schrödinger equation and the size of basis sets.

> *Semi-empirical pseudopotentials have been used to calculate electronic energies and lifetime of charge carriers in large structures (10-100nm) with up to millions of non-equivalent atoms (HIPERSOL).*

1.2.3 Semi-empirical tight binding potential (TB) model

The opposite extreme to the nearly-free electrons is the case where the electrons in the crystal are tightly bound and behave much like the atoms. The tight binding model (TB) is an atomistic approach to the calculation of electronic band structure where electronic states are written as linear combinations of atomic orbitals centered in the atomic nuclei. The method is closely related to the

LCAO method used in ab initio models. Electrons are viewed as occupying the standard orbitals of their atoms, and then 'hopping' between atoms during conduction.
Tight binding models are applied to a wide variety of solids. The approximation works well in materials with limited overlap between atomic orbitals and limited overlap between potentials on neighbouring atoms. Band structures of materials like Si, GaAs, GaN, SiO_2 and diamond for instance are well described by TB-Hamiltonians.

This model can be used to perform finite-temperature simulations, and calculate thermoelectric properties and electronic transport calculations (OXIDES), to evaluate hydrogen trapping at extended crystal defects such as grain boundaries and dislocations (MULTIHY) to explore effects connected to finite temperature and disorder (ATHENA) and to describe electronic and optical properties of GaN based nanowires (SMASH)

1.2.4 Hubbard model

The Hubbard model is the simplest model of interacting particles in a lattice, with only two terms in the Hamiltonian: a kinetic term allowing for tunneling ('hopping') of particles between sites of the lattice and a potential term consisting of an on-site interaction, which stems from the Coulomb repulsion between electrons occupying the same atomic orbital. For electrons in a solid, the Hubbard model can be considered as an improvement on the tight-binding model, which includes only the hopping term. The Hubbard model is actually the simplest model able to describe the interaction-driven transition from a metal to an insulator, commonly known as the Mott transition. Mott insulators are commonly found within transition metal oxides and organics, where the Coulomb repulsion overwhelms the very narrow bandwidth. More recently, the Bose- and Fermi-Hubbard models has been used also invoked to describe the behavior of ultra-cold atoms trapped in optical lattices. The Hubbard model is a good approximation insofar the effect of all other bands but the conduction ones can be neglected, which corresponds to low enough temperature and energy so that all interband transition are uninfluential. If interactions between particles on different sites of the lattice are included, the model is often referred to as the 'extended Hubbard model'.

The fact that the Hubbard model cannot be solved analytically in arbitrary dimensions has led to intense research into numerical methods for strongly correlated electron systems.

The Hubbard model can also be studied within the Monte Carlo statistical method for example to study the electronic exchange interaction in non-equilibrium situations (FEMTOSPIN). Molecular Hubbard models for ground state and low temperature properties of strongly correlated materials have been used to calculate long ranged electron-electron interaction and insulator-superconductivity transitions in lattices under pressure (LEMSUPER) and to model the Hamiltonian of inorganic metal nanoparticles embedded in matrices of conjugated organic materials (HYMEC).

1.2.5 k·p effective Hamiltonian

This is a technique that allows a band structure to be approximately described in terms of just a few parameters. The technique is commonly used for semiconductors, and the parameters in the model are often determined by experiment.

This model can be used to calculate conduction and valence band edges and effective masses of the charge carriers. Thereafter these values can e.g. be used as input to a drift diffusion model calculating the electron and hole transport (SMASH) or to micromagnetic models for magnetisation (NAMASTE).

1.2.6 Polarisable continuum model

The polarisable continuum model (PCM) is commonly used to model a solvent-mediated chemical reaction. If it were necessary to consider each solvent molecule separately, the computational cost of modeling would grow prohibitively high. Instead the solvent reaction field is simulated by a set of apparent charges self-consistently determined on the basis of the electric potential generated by the solvated molecules.

This model has been used to simulate the effect of surrounding solid electrolyte weakly interacting with the conductive molecules in excitonic solar cells (INNOVASOL).

1.2.7 Envelope function approximation for continuous media

The wavefunction varies very quickly close to the cores of the atoms of the lattice. The *envelope approximation* means that only the slowly varying "envelope" modulating the rapidly varying part of the wavefunction is considered. The boundary conditions are applied to the envelope function directly, rather than to the complete wavefunction.

This method is used to calculate the quantum states of confined particles in nanostructures (SMASH).

1.3. Quantum mechanical in response to time dependent fields

To study electronic and spin dynamics under the effect of external time dependent potentials, such as electric or magnetic fields, time dependent models are needed.

1.3.1 TD-DFT and TD(Spin)DFT

Time-dependent density functional theory (TDDFT) is a quantum mechanical model used to investigate the properties and dynamics of many-body systems in the presence of time-dependent potentials, such as electric or magnetic fields. The effect of such fields on molecules and solids can be studied with TDDFT to extract features like excitation energies, frequency-dependent response properties, and photo-absorption spectra.

As TDDFT is an extension of DFT, the conceptual and computational foundations are analogous and use the effective potential of a fictitious non-interacting system which returns the same density as any given interacting system. Numerically, this TDDFT model is much more complex then DFT, most notably because the time-dependent effective potential at any given instant depends on value of the density at all previous times. Note however that at present most of the implementation assume a local time-dependence of the potential (adiabatic approximation).

TDDFT is able to account correctly for magnetic fluctuations in the paramagnetic state of iron and other itinerant ferromagnets, the effects of vibrations (electron-ion dynamics) on photo-energy conversion (CRONOS, INNOVASOL) and it is used to calculate transport properties in systems with a strong correlation term between particles (HYMEC).

If needed, the equation of motion for the spin degrees of freedom can be derived with time-dependent spin-density-functional theory ,TD-SDFT, which includes the spin density interacting with the external magnetic field. This can then be used to calculate non-linear interactions between spin, conducting electrons and laser light (FEMTOSPIN and CRONOS).

1.3.2 The time-dependent k·p-model

This quantum kinetic model describes the time evolution of the multi-band electronic state and is a linear coupled system of Schrödinger equations. The evolution is governed by the k·p Schrödinger operator which as an extension to the single-band models describes a system of bands of the band structure, usually the four topmost valence bands.

1.3.3 Other time-dependent models

The time-dependent approach based on the Gutzwiller wave function and approximation is a very simple tool that allows simulating for quite long times the non-equilibrium evolution of correlated electron models. It is in essence an improvement of the time-dependent Hartree-Fock approximation, endowing a Hartree-Fock Slater determinant with local many-body correlations that better capture the collective nature of the Mott localization phenomenon. It is a rigorous variational approach in the limit of large lattice-coordination, but seems to provide qualitatively correct results also beyond that limit.

The time-dependent Gutzwiller approach is able to model the temporal evolution of correlated materials brought out-of-equilibrium by ultra-fast laser pulses (GOFAST).

The Blonder-Tinkham-Klapwijk model is used to describe the normal-superconducting microconstriction contacts at the crossover from metallic to tunnel junction behavior. The Blonder-Tinkham Klapwijk (BTK) model in its simplest form does not require any input from other models. In its 3D extension, the BTK model requires in input the shape of the Fermi surface. In any case, this model allows fitting the gap features of the point-contact Andreev-reflection (PCAR) spectra and thus obtaining the amplitude and the symmetry of the superconducting gap(s).

The multiband Eliashberg theory includes interband spin-fluctuation interactions and describes superconductivity-induced infrared optical anomalies. The multiband Eliashberg model requires some input from band structure calculations (normal DOSs at the Fermi levels) and contains 2 free parameters (namely the coupling strengths) that can be adjusted to reproduce the gaps provided by the BTK fit of the spectra and the experimental critical temperature.

In particularly good contacts, the point-contact spectra also contain electron-boson structures that cannot be fitted by the simple BTK model; in these cases, since one of the outputs of the Eliashberg model is the whole energy-dependent gap function, this may be put in the extended BTK model to calculate theoretical point-contact spectra that feature electron-boson structures that can be compared to the experimental ones.

These models have been used to calculate the intrinsic physical parameters (superconducting transition temperature, penetration depth, upper critical field) and superconductance energy gaps (IRON SEA), which are very important intrinsic physical parameters in superconductors..

1.4. Electron transport model

1.4.1 Semi-classical drift-diffusion model

This is a popular semi-classical model to describe the transport of charge carriers in solids, and especially useful for semiconductors. It consists in writing classical equations for the carrier current in terms of the electrochemical potential.

The carrier density distribution is modelled using quantum mechanical Fermi-Dirac statistics or Boltzmann statistics.
The necessary input parameters like band gap, carrier mobility and diffusion coefficient are obtained empirically or with separate theoretical calculations, using the Einstein relation.

Several assumptions are made: non degeneracy, charge conservation, local equilibrium, and constant temperature.

The drift diffusion model has been used to simulate electronic transport in large diameter hetero-junction nanowires with tunnel junctions (AMON-RA), to calculate electron transport across oxides interfaces (MORDRED), electron and holes transport in Gallium Nitride based nano-rod structures (SMASH) and to calculate steady state conductivity (high and low state) in organic semiconductor device (HYMEC).

Chapter 2
Atomistic models

Most molecular systems and phenomena of interest in physics and chemistry are too large to be treated by quantum mechanics simulations, even if semi-empirical approximations are used. Atomistic models aim at simulating the behaviour of larger molecular systems (typically between 10^2 and 10^9 atoms, length scale 0.1-100nm, timescale fs-μs) maintaining individual atomistic detail, but often removing an explicit representation of the electrons. Although these systems are not large enough to be considered macroscopic, they are often sufficiently large to reproduce experimental results within the desired accuracy and at the same time detailed enough to detect their microscopic origin.

These large assemblies are too large to be described in a deterministic way, and atomistic simulations are thus based on statistical mechanics, statistical thermodynamics and other probabilistic theory. They consist in treating the many-atoms system as a large statistical population, whose time evolution is determined by the forces applied to each single atom. Statistical mechanics provides the mathematical framework for relating the microscopic properties of individual atoms and molecules to the macroscopic bulk properties of materials that can be observed in everyday life. These models explain macroscopic structural and dynamical observables (e.g. temperature, pressure, work, heat, free energy, entropy and spectra of these variables) based on classical and quantum-mechanical descriptions of statistics and mechanics at the microscopic level. For example, a macroscopic observable like temperature is due at microscopic level to the collisions between particles and can therefore be mathematically derived sampling the velocities of the atoms.

For the statistical mechanics formulation to be valid, the averaging has to be done over all possible configurations of the system, i.e. all possible positions and momenta of all particles (ergodic condition). This is true if the simulation is infinitely long, and approximately true if the system is allowed to evolve for a sufficient amount of time. The ergodic condition may be more difficult to achieve in systems with many degrees of freedom, or with large energy barriers between possible configurations, as the systems may be trapped in one local energy minimum. Methods to overcome this problem and speed up the configurational sampling are an active field of research.

To determine whether or not to use continuum models or statistical mechanics, the Knudsen number may be evaluated for the problem. The Knudsen number is defined as the ratio of the molecular mean free path length to a certain representative physical length scale. This length scale could be, for example, the radius of a body in a fluid. More simply, the Knudsen number is how many times its own diameter a particle will travel on average before hitting another particle. Problems with Knudsen numbers at or above unity are best evaluated using fine scale (atomistic and mesoscale) statistical mechanics for reliable solutions.

In general, atomistic models have to answer two fundamental questions:

1. How can the interactions between the atoms be described?

2. What equations are used to obtain the macroscopic proprieties that can be compared with experiments?

First the first question is addessed and interatomic potentials and force fields are discussed in paragraph 2.1. In paragraph 2.2-2.5 three different sets of equations will be discussed: molecular dynamics, Monte Carlo molecular models and atomistic spin models.

2.1 Interatomic potentials

2.1.1 Force Fields and Molecular Mechanics

If the full Schrödinger equation for all atoms can't be solved, it is crucial to develop models for interactions between the atoms, since these play a crucial role in determining the behaviour of a system. This can be done in the form of the interatomic potentials.

In molecular simulations, the interatomic potential is usually represented by simple analytical parametrical expressions. Interatomic potential functions and parameter sets can be derived from both experimental work and quantum mechanical calculations for a small number of appropriate test molecules. Validation of parameter sets is done against experimental results on larger and more diverse systems. This is done to ensure transferability of parameters across a diverse range of systems and test the accuracy limits of the parametrisation. Optimisation of existing potentials and development of new potentials is a very active field of research.

> *New interatomic potentials for atomic simulations have been developed for tungsten and various oxides (ADGLASS), for zeolitic imidazolate frameworks (ZIF-8 crystals) (AMCOS), and for selected metal alloys (MINTWELD).*
>
> *A novel interatomic potential for Cu_2O has been also developed to conduct the analysis of Cu (111)/ Cu2O (111) interfacial failure and is based on a combined Lennard Jones - Morse parameterized interatomic potential (NANOINTERFACE).*

A force field is a system of interatomic potential energy functions and parameters used in molecular mechanics simulations.

In all-atoms force fields, each atom is represented explicitly, including the light and small hydrogen, while in united-atom force fields some atoms, like hydrogen and carbon atoms in methyl and methylene groups, are treated as a single unit. Grouping of larger atomic moieties may be necessary to simulate larger systems for longer times and this is treated in the next chapter under coarse-grained mesoscopic models. Typically, first each atom is modelled by aligning it a radius (usually the van der Waals radius), a polarisability, and a constant net charge (generally derived from quantum calculations and/or experiment).

The next step is to model the force field. Force fields usually consist of a sum of additive terms, which represent both bonded interactions (between atoms that are actually covalently bonded) and non-bonded interactions. Terms between bonded atoms include: bond terms between 2 atoms, bend terms between 3 atoms, and torsional (dihedral) terms between 4 atoms. Bond and bend terms are treated as springs with an equilibrium distance equal to the experimental or calculated value. For

accurate reproduction of vibrational spectra, the Morse potential can be used instead, at higher computational cost. The dihedral or torsional terms have multiple minima and cannot be modeled as springs, and their specific functional form varies in different force fields. Additionally, "improper torsional" terms may be added to enforce the planarity of aromatic rings and other conjugated systems, and "cross-terms" may be added that describe coupling of different internal variables, such as angles and bond lengths. Some force fields also include explicit terms for hydrogen bonds.

The non-bonded terms are much more computationally costly to calculate in full, since a typical atom is bonded to only a few of its neighbors, but interacts with every other atom in the system. The electrostatic force between nuclei and charged particles is a typical non-bonded interaction and is given by Coulomb's law. Long-range electrostatic interactions are often important features of the system under study (especially for proteins) but the electrostatic terms are notoriously difficult to precisely calculate well because they do not fall off rapidly with distance. A variety of methods are used to address this problem; the simplest approximation consists in using a cut-off range for these interactions and atom pairs whose distances are greater than the cutoff have a van der Waals interaction energy of zero.

Other more sophisticated but computationally intensive methods are known as particle mesh Ewald (PME) and the multipole algorithm. To account for electronic polarisability and produce better agreement with experimental observations, parameters can be buffered or scaled by a constant factor.

Other non-bonded forces are London dispersive interatomic forces (attractive) and electron-electron short range forces (repulsive). These are typically modelled together using the so-called Lennard-Jones potential.

Notwithstanding their simplicity, force fields can reproduce quite well a wide variety of chemical and biological problems, including drugs binding, protein folding kinetics and protonation equilibria.

2.1.2 Bond Order Potential Model (BOP)

Bond order potentials belong to a class of empirical analytical potentials which is used in molecular simulations. Examples include the Tersoff potential, the Brenner potential, the Finnis-Sinclair potentials, ReaxFF, and the second-moment tight-binding potentials. They have the advantage over conventional molecular mechanics force fields in that they can, with the same parameters, describe several different bonding states of an atom, and they may thus, to some extent, be able to describe chemical reactions correctly. The potentials were developed partly independently of each other, but share the common idea that the strength of a chemical bond depends on the bonding environment, including the number of bonds and possibly also angles and bond length.

This model has been used to calculate effective hydrogen diffusivities under different defects distribution, stress/strain and temperature conditions (MULTYHI).

2.2 Molecular Dynamics (MD)

What equations can be used to obtain the macroscopic proprieties that are then compared with experiments?

The equations used in Molecular Dynamics to obtain macroscopic properties are the equations of motion for all atoms in the system. Molecular Dynamics consists in simulating molecular trajectories by integrating the equations of motion. The time duration of the simulation is broken down in small time steps. Using a numerical integration scheme, the dynamics of each atom in the system under the effect of the interatomic forces is calculated for each time step.

The length of the time step chosen is a compromise between a value large enough to allow a reasonably long simulation time for the purpose of the study and a value small enough to capture all the required fundamental frequencies of motion in the system and conserve the energy between integrations steps. Typically this is in the range of 1-10 fs, but depends on the range of motions allowed in the system. Multiple time scale calculations, where rapidly changing forces are updated more frequently than slowly changing forces, are also possible in order to reduce the required computational time.

Large systems which are repetitive at a certain scale can be simulated using periodic boundary conditions. In these, forces are calculated only for atoms contained in a unit cell and then replicated across 1, 2 or 3 dimensions to simulate the effect of particles entering and leaving the unit cell. The size of the unit cell needs to be large enough so that each particle does not feel the influence of its mirror image in one of the replicated cells.

Temperature and pressure can be controlled using numerical methods that simulate the effect of a thermostat or barostat or using stochastic methods like Langevin dynamics that add friction and random forces to account for molecular collisions.

The main advantage of molecular dynamics with respect to other molecular simulation methods is that not only does it allow obtaining macroscopic properties (e.g. temperature, pressure, work, heat, free energy, and entropy) that can be compared with experiment, but also the trajectory of the system during the simulation from which dynamical and structural quantities can be obtained.

Simulations with molecular dynamics can reproduce conditions in real life experiments and even experiments that are not possible, safe or wise to perform.

2.2.1 Classical Molecular Dynamics

Molecular Dynamics (MD) calculations performed using force fields and integrating the classical Newton's equations of motions for atoms are called classical MD. Several software packages are available (see Annex II) and several implement their own force field.

Classical molecular dynamics has been used to model morphological properties of solar cells, light emitting diodes, transistors, batteries and ultra capacitors. They are used to generate the Si/Ag and Si/Ni interfaces accounting for strain and misfit dislocations to investigate influence of N content and gradients on the trap density at the interface (HIPERSOL).

Classical molecular dynamics has also been used to calculate the interface dipole at organic/organic interface (MINOTOR), to predict the bulk organization and simulate realistic interfaces between the insulating layer and the organic semiconductor at the nanometre scale (ONE-P).
Classical molecular dynamics has been used to calculate physical properties of nanostructured materials (MONAMI), to calculate dynamic charge transfer in nanoelectronics devices (MORDRED) and to calculate properties of branched polymers as host matrices for Li-ion battery solide polymer electrolytes (SUPERLION).

Classical molecular dynamics has been extensively used to study interface problems in matrices, composites, coatings, cracks and defects structures. In particular, it has been used to determine average confirmation, chain stiffness, degree of counterion condensation of polyelectrolyte chains, formation of surfactant polyelectrolyte complexes and adsorption of single electrolyte chains, formation of polyelectrolyte layer (MUST), to study large scale defect structures in the ceramics such as dislocation and incoherent grain boundaries (ROLICER), to calculate strength of hydrogen bonding and dispersion interactions and adsorption of water or carbohydrate in cellulose surfaces (SURFUNCELL). In surface engineering of reinforced and nanostructured composite and polymers, classical molecular dynamics has been used to simulate the effect of functionalization of the mechanical properties of the CNT and calculate the stress strain slope as well as the interfacial interactions between CNTs and polymeric matrices (POCO), to extract local traction and crack opening displacement data and calculate densities, glass transition temperature, volumetric coefficient of thermal expansion and isotropic mechanical properties to validate the simulation of the polymer network formation in the epoxy resin (NANOINTERFACE). In hydrogen storage and fuel cells development, it has been used to simulate adsorption in proton exchange membranes (HYPOMAP).

2.2.2 Ab initio molecular dynamics

With the progress of computational speed and memory, it is possible to perform calculations of Molecular Dynamics which take into consideration explicitly the effect of the electrons in the calculation of the forces (ab initio MD). Although still limited to smaller systems and shorter periods of time than classical MD, a significant advantage of using ab-initio methods is the ability to study, without empirical parameters, reactions that involve breaking or formation of covalent bonds, tunneling and proton transport mechanisms.

The main challenge consists in calculating efficiently and accurately the forces acting on the nuclei due to the electrons. Since many electrons are in the system their potential energy is represented by a multidimensional surface for each nuclei configuration. Assuming that it is possible to decouple the motion of the electrons from the motion of the nuclei (Born-Oppenheimer approximation), the classical equations of motion for the nuclei are integrated using the sum of the interatomic potential and the forces derived from the electron potential energy surface. At each time step, the ground-state electronic potential surface can be calculated using standard quantum mechanical methods (Born-Oppenheimer Molecular Dynamics) or introducing fictitious dynamics for the electrons which follow adiabatically the nuclei and are subjected to small readjustments "on the fly" during the nuclei evolution to keep them close to the ground state potential surface **(**Car-Parinello Molecular Dynamics).

Ab initio MD has been used to calculate pressure induced metallisation of potential high pressure superconductors (LEMSUPER), to calculate ab initio surface and interface energies in metal alloys and electric active materials (MINTWELD), and to calculate magnetic properties, solvatochromism, non-linear optical properties, like hyper-polarisability and two-photon absorption of large solvated systems including more than 10,000 atoms (MONAMI).

2.2.3 Quantum mechanics/molecular mechanics (QM/MM)

For systems in which full consideration of electrons is not feasible, it may still be possible to perform calculations that retain some quantum mechanical details. Quantum Mechanical/Molecular Mechanics methods (QM/MM) consist in finding a working subdivision of the system into a part that needs to be calculated at quantum mechanical level and a (larger) part that can be calculated using classical force fields based molecular dynamics, the molecular mechanics part. For example, a QM/MM scheme can be used to calculate the reactions occurring between a drug and the target protein binding site atoms, while the rest of the protein is simulated with classical molecular dynamics. The challenge is to define the forces at the interface between the region treated with QM and the region treated with MM.

ONIOM-like scheme (DFT/MM) have been used to simulate the formation energy of inclusion complexes in layered magnesium oxides, relevant for the synthesis of quasi-solid electrolytes to be used in solar cells and binding energy of the different crystallographic phases to organic passivants (INNOVASOL).
QM/MM has been used to calculate the adhesion of proteins at the interface between a glassy SiO2 phase and a water solution, relevant to pharmaceutical applications and the cohesion between a glassy SiO2 phase and crystalline TiO2 phases, relevant to thin-layer-based conditioning of glass materials for applications in architectural glass and photovoltaic cells (ADGLASS).
DFT/MM gives reaction paths and relative energies of stationary points in organic-based electronic devices (MINOTOR).

2.3. Statistical Methods (Monte Carlo molecular models)

In the mathematical framework of statistical mechanics, it is not necessary to follow the dynamics of the systems to calculate macroscopic observables. These are in fact derived from an accurate sampling of all equivalent microscopic configurations of the system.

Monte Carlo (MC) methods are statistically based methods. They generate non-sequential configurations of the system according to appropriate Boltzmann probabilities for the system. The model employs the Metropolis algorithm and Markov chain protocol in order to determine a new state for a system from a previous one. The new configuration is then accepted or rejected on the basis of importance sampling criteria.

Then macroscopic observables (e.g. temperature, pressure, work, heat, free energy, and entropy) are calculated from the positions of the atoms in all configurations sampled, even if each subsequent configurations are not connected with each other in time.

With MC models the sampling efficiency can be increased, which is particularly important where the potential surface contains many local minima (as in close to state transitions, in large proteins etc).

The success of this method in statistical mechanics has led to various generalisations, such as the method of simulated annealing for energy optimisation of a system, in which a fictitious high temperature is introduced to obtain a fully random sample and then gradually lowered to obtain a configuration close to the ground state. Hybrid Monte Carlo methods introduce an acceptance criterion into molecular dynamics simulations, allowing the use of large time steps. Kinetic Monte Carlo methods apply the same statistical principles to simulate the time evolution of the processes under consideration. Typically these are processes that occur with a given known rate and the rates with which these processes evolve are inputs to the KMC algorithm, the method itself cannot predict them.

Monte Carlo based methods have been used to predict the sorption isotherms in the investigated materials: zeolitic imidazolate frameworks, hyperbranched aminosilicas, and functionalised polymers (AMCOS), to study the aggregation of C-S-H particles growth of microstructure using macroscale parameters (CODICE), to calculate diffusivities of charge carriers and band structure for up to 10000 atoms (HIPERSOL), to calculate charge carrier propagation and density in the doped layer (MINOTOR), to calculate statistical variability of electrical impact of defects (MORDRED). Kinetic Monte Carlo models have been used to calculate charge propagation and charge carrier mobility, to quantify the impact of different dielectrics on the charge carrier mobility and the exciton diffusion length (ONE-P); and to follow the evolution of individual defects to calculate irreversible processes at atomic scale under irradiation conditions (RADINTERFACES).
Monte Carlo method was also used to solve the Boltzmann transport equation for the description of gas flow and plasma to calculate particle motion, interaction between phases, and transport proprieties in oxide based electronic materials (ORAMA).

2.4. Atomistic spin models

Spin models are used to describe magnetic material properties. A spin here normally represents the magnetic moment of an atom, the energy of which is typically parameterized within a Heisenberg formalism, though even relativistic interactions, like Dzyaloshinskii-Moriyam interactions or anisotropies can be taken into account. The fact that magnetic structures are described on an atomic level allows for an investigation of ferromagnets as well as ferrimagnets and antiferromagnets or even heterostructures composed of different materials.

In the classical limit the equation of motion is the Landau-Lifshitz-Gilbert (LLG) equation.
The LLG equation describes the spin precession that follows from Heisenberg's equation of motion and its relaxation into an equilibrium direction via a damping term (either after Landau and Lifshitz or after Gilbert) with a corresponding damping parameter. Though the LLG equation is partly phenomenological this approach turns out to be very successful.
When augmented by a stochastic term to introduce Langevin dynamics it allows for the calculation of thermal equilibrium and non-equilibrium properties of magnetic systems where the heat-bath can be provided by phononic or electronic degrees of freedom. With that

approach equilibrium properties like phase transition can be described and investigated as well as ultra-fast phenomena as, e.g., optically induced switching events.

Currently, up to 10^8 spins can be treated numerically, for 2-D structures corresponding to up to 1000nm length scale, and up to some nano seconds time scale.

This model has been used to calculate dissipation channels and energy transfer in order to identify optimal materials for ultrafast optically induced magnetic switching and the relevance of the specific spin ordering in ferro-, ferri-, antiferro-magnetic and magnetic semiconductors (FEMTOSPIN).

2.5 Semi-classical non-equilibrium spin transport model

Irradiation of a ferromagnetic metal layer with a femtosecond laser pulse causes a sudden demagnetization within a few hundred femtoseconds. While this discovery holds potential for an "ultrafast" revolution of existing hard disk technology, the underlying physical mechanism of ultrafast laser-induced demagnetization could not yet be uncovered. Computational modelling is needed to unravel the various possible contributions to the demagnetization processes.

A model to describe the laser-induced non-equilibrium transport occurring on the nanoscale has been developed. The model treats explicitly the laser-created distribution of highly energetic, spin-polarized electrons, which immediately start to move randomly through the material (typical velocities of several nm/fs). These hot non-equilibrium electrons undergo random scattering with other electrons or with phonons and thereby they loose energy, i.e., the process of electron thermalization. Solving numerically the derived transport equation, using spin-lifetimes taken from *ab-initio* calculations, reveals that laser-excited hot electron transport occurs neither in the diffusive nor ballistic regime, it is superdiffusive. Moreover, as spin-majority and minority electrons have distinct lifetimes, fast spin-dynamics on the femtosecond time scale is generated.

Notably, superdiffusive transport of mainly spin-majority electrons causes an ultrafast demagnetization of the ferromagnetic layer. The modelled time-dependent magnetization $M(t)$ of a 17 nm Ni layer on Al is in good agreement with the measured demagnetization, which exemplifies that ultrafast spin-transport acts as a mechanism for laser-induced demagnetization.

Multiscale modelling of ultrafast spin-dynamics is performed in FEMTOSPIN. To comprehensively model the various spin-dynamical processes, occurring on different length- and time-scales, different computational approaches are needed. FEMTOSPIN is using the non-equilibrium spin transport model to simulate the laser-induced hot electron transport on the femtosecond time-scale, treating magnetic layered heterostructures with a total layer thickness of about 100 nm.

Chapter 3
Meso-scale models

Meso-scopic models address 10^6 up to unlimited number of atoms, length scales of 100nm-mm and timescales of ms-s. They can be based on their equivalent atomistic equations. Molecular models belong to this class if they group more than one atom together in order to allow simulation of larger systems and for longer times, although in so doing they loose some of the atomistic details.

Also micro-magnetics is classified in this group due to the scales addressed (length scale 1 nm - 100 mm, timescale 1ps-1000ns). Note that scientists, coming from continuum physics, call this area "micro", but in the large constellation of models addressing materials, this scale is intermediate and called 'meso'.

Even if the mathematical details of many models may be similar to the ones already discussed and don't need to be repeated here, some implications and unique aspects of meso-scopic models will be highlighted in this Chapter.

3.1. Statistical meso-scopic models

Monte Carlo molecular models can be applied at a meso-scopic level, but no specific aspects of the model need to be added to those already discussed.
Lattice gas automata (LGA) or lattice gas cellular automata (LGCA) models are used to simulate diffusion. It was the precursor to the lattice Boltzmann models. From the LGCA, it is possible to derive the macroscopic Navier-Stokes equations (see Ch 4.2). These models comprise of a lattice, where the sites on the lattice can take a certain number of different states. The various states are 'particles' with certain velocities. Evolution of the simulation is done in discrete time steps. After each time step, the state at a given site can be determined by the state of the site itself and neighboring sites, *before* the time step. The state at each site is purely Boolean. At a given site, there either *is* or *is not* a particle that is moving up. At each time step, two processes are carried out, propagation and collision. In the propagation step, each particle will move to a neighboring site determined by the velocity that particle had. Barring any collisions, a particle with an upwards velocity will after the time step maintain that velocity, but be moved to the neighboring site above the original site. The so-called exclusion principle prevents two or more particles from travelling on the same link in the same direction.
In the collision step, collision rules are used to determine what happens if multiple particles reach the same site. These collision rules are required to maintain mass conservation, and conserve the total momentum; the block cellular automaton model can be used to achieve these conservation laws. Note that the exclusion principle does not prevent two particles from travelling on the same link in *opposite* directions. When this happens, the two particles pass each other without colliding. Macroscopic quantities like the density at a site can be found by counting the number of particles at each site. If the particles are multiplied with the unit velocity before being summed, one can obtain the momentum at the site. However, calculating density, momentum, and velocity for individual sites is subject to a large amount of noise, and in practice, one would average over a larger region to obtain more reasonable results. Ensemble averaging is often used to reduce the statistical noise further.

Kinetic Monte Carlo and lattice gas automata have been used to calculate diffusive transport and sorption of carbon dioxide (AMCOS), to simulate the release of the healing agent from micro-containers and its propagation during self-healing action (MUST) and to calculate charge and mass transfer (SUPERLION).
Kinetic meso-scopic Monte Carlo has been used to evaluate effective H diffusivities under different strain conditions and trap densities and temperature (MULTIHY).

3.2. Meso-scopic particle-based models

Coarse-grained Molecular Dynamics

Coarse-grained Molecular Dynamics is a particular kind of classical molecular dynamics where a force field is developed for a group of atoms as large single unit, also called pseudo atom.
The simplest form of coarse-graining is the "united atom" (sometimes called "extended atom") and was used in most early MD simulations of proteins, lipids and nucleic acids. For example, instead of treating all four atoms of a CH_3 methyl group explicitly (or all three atoms of CH_2 methylene group), one represents the whole group with a single pseudo-atom. This pseudo-atom must, of course, be properly parameterized so that its van der Waals interactions with other groups have the proper distance-dependence. Similar considerations apply to the bonds, angles, and torsions in which the pseudo-atom participates. In this kind of united atom representation, one typically eliminates all explicit hydrogen atoms except those that have the capability to participate in hydrogen bonds ("polar hydrogens"). This approximation can provide substantial savings in computer time as coarse-grained models can provide a simpler representation of nucleotides and acids which are large molecular units for the simulation of larger systems: DNA/RNA strands, long chain polymer, membrane lipids and proteins.
The mathematical challenge is in the calculation of the forces, in the determination of the pseudo-atoms charge distribution and in the parametrisation of these coarser-grained potentials.

Coarse grained models are used to describe the competition between cohesive and adhesive failure and cross-linked models of epoxy networks (NANOINTERFACE) and to study the structure and dynamics of silica-polystyrene nanocomposite systems (NANOMODEL). Particle-based coarse-grained models have also been used to calculate the flow of latex particles to obtain semi-quantitative predictions of linear and non-linear rheology (MODIFY) and the formation of layers of nanoparticles on cellulose surfaces (SURFUNCELL).

Discrete lattice model

An alternative to coarse-grain simulations in solids is to use an atomic finite element model (discrete lattice model). This consists in using units like bars, or trusses, just like the elements in a standard finite element analysis. The behaviour of the bar is described by an interatomic potential. This enables an atomic lattice to be modelled by an assemblage of members that deform according to a prescribed interatomic potential, which governs their relative separations under applied loading. A key feature of the atomic finite element model is that it results in a finite element equation with

displacement degrees of freedom. An atomic finite element mesh can be directly coupled to other element types and to find element models at larger scales.

3.3. Micromagnetic models

Micromagnetics deals with the interactions between magnetic moments on sub-micrometre length scales. The underlying assumption is that the spins at electronic and atomic level are coupled to one "macro-spin". These interactions are described by several competing energy terms. Exchange interaction (responsible for the very existence of ferro- and antiferromagnetic materials) 'attempts' to align adjacent magnetic moments (in ferromagnetic materials) or antiparallel (in antiferromagnetic materials). Magnetodipolar contribution accounts for the energy of a magnetic moment in the (dipolar) field created by all other moments of a magnetic body. Anisotropy energy is mainly due to the spin-orbit interaction and the anisotropy of the crystal lattice: it is low when the magnetic moments are aligned along a particular crystallographic direction. Zeeman energy describes the interaction between magnetic moments and external magnetic field and is at its lowest when the moments lie parallel to this external field. The competition of these interactions under different conditions is responsible for the overall behavior of a magnet.

Since the equilibrium arrangement of magnetic moments ("magnetisation configuration") is usually (but not always!)the one in which the total magnetic energy is lowest, the sum of these four energy terms will 'attempt' to become as small as possible (with some energy terms decreasing at the expense of the others), yielding complex physical interactions.

A form of the Landau-Lifshitz-Gilbert equation is used to solve time-dependent micromagnetic problems. An essential merit of the micromagnetic theory concerns the answer to the question, how the effective magnetic field depends on the relevant
Usually the exchange interaction and the magnetic dipole-dipole interaction term play the dominating role, usually a *competing* one. In particular: due to the last term the effective field is a *nonlocal* function of the magnetisation, i.e. although the Landau-Lifshitz-Gilbert equation looks relatively harmless, one is actually dealing with a complicated nonlinear set of integro-differential equations.
The necessary material constants can either come from measurements or from electron-spin and atomistic ab-initio models.

DYNAMAG is using micromagnetics OOMFF , NMAG and DGCA models for spin dynamics including spin transfer and anti-ferromagnetic and ferromagnetic sub-lattices interactions.

FEMTOSPIN is using micromagnetics model called 'Madrid/Konstanz code' to predict the behaviour of ferrimagnetic and anti-ferromagnetic materials and magnetic semiconductors for heat assisted recording.

MAGNONICS uses several micromagnetic codes (finite-difference codes MicroMagus and OOMMF and a finite-element package Nmag) to compute magnetization reversal processes and pico- and nanosecond magnetization dynamics in structured arrays of magnetic nanoelements.

MASTER is using a micromagnetics model based on the Landau-Lifshitz-Gilbert equation called SPINPM to predict magnetisation dynamics in an array of hetero-structures.

NAMASTE is using an in-house micromagnetics code to calculate magnetisation, relativistic magneto-crystalline anisotropy constants, gilbert damping coefficients and magneto-resistance coefficients of metals and magneto-transport properties of ferromagnetic semiconductor nanostructures.

REFREEMAG is using micromagnetics dynamic models based on Landau-Lifshitz-Glibert equation called FEMME and MAGPAR to calculate the shape anisotropy and hysteresis properties of meso-scopic magnetic structures including coercive field and switching times. Also the thermal stability depending on geometry and the size of the magnetic volumes is calculated.

SSEEC is using a micromagnetics model to provide the exchange coupling at nano-scale between "particles" in a composite (meta) material.

ULTRAMAGNETRON has used a micromagnetics code based on the LLBloch equation at nm scale taking the exchange coupling as well as the dipolar interaction into account to calculate magnetisation at elevated temperatures and the dynamics of ferrimagnetic materials.

Chapter 4
Continuum modelling of materials

Parts of this text have been taken from Wikipedia

This chapter concerns with designing materials with desired continuum scale properties. Modeling for materials design is about investigation of relations between chemical composition, microstructure and effective properties.

Materials, such as solids, liquids and gases, are composed of molecules separated by empty space. Physical and chemical processes at the smallest scale are modeled by electronic and atomistic models as addressed in Chapter 1 & 2. However, certain physical phenomena can be modeled assuming the materials exist as a continuum, meaning the matter in the body is continuously distributed and fills the entire region of space it occupies. A continuum is a body that can be sub-divided into infinitesimal elements assuming that the substance of the object completely fills the space it occupies. The element is assumed to have the properties of the bulk material. In these elements the processes at smaller scale are averaged out. Many physical phenomena are multi-scale in nature and researchers must look to multi-scale methods that couple electronic, atomistic and continuum simulations. This linking will be addressed in Chapter 6. In this Chapter continuum models will be described.

The length scale for continuum modelling has two limits: the lower limit is related to the notion "continuum" and this lower limit is much bigger than a molecule; the upper limit is related to the requirement that the model adequately describes reality and this upper limit is thus smaller than any spatial variation in material properties. When the spatial variation length scales are not much greater than that of inter-atomic distances or when a continuum of a finer resolution is to be established statistical mechanics is used (see Chapter 3) and modellers employ statistical volume elements and random continuum fields linking continuum mechanics to statistical mechanics. Specifically for fluids, the Knudsen number is used to assess to what extent the approximation of continuity can be made.

In continuum modeling it is possible to apply a chain of modelling that uses the same physics and chemistry equations applied to different scales. Often the modeling at a smaller scale is called "micro-modeling" and the results of these models are, after being homogenised, fed into "macro-models" in the form of new macroscopic constitutive equations (a concept that will be elaborated below).

This chapter will deal with

4.1 Continuum mechanics (solids and fluids)
4.2 Chemistry
4.3 Electromagnetism

The text has been rigorously organised along the concepts

- Fundamental physics and chemistry laws (conservation equations) forming the model
- Material specification in constitutive equations and constraints

4.1 Continuum mechanics

The parts of continuum mechanics addressed in material science and technology are:

<table>
<tr><td rowspan="3">Continuum mechanics

The study of the physics of continuous materials (Chapter I)</td><td rowspan="2">Solid mechanics
The study of the physics of continuous materials with a defined rest shape.</td><td colspan="2">Elasticity and visco-elasticity
Describes materials that return to their rest shape after an applied stress.</td></tr>
<tr><td>Plasticity
Describes materials that permanently deform after a sufficient applied stress.</td><td rowspan="2">Rheology
The study of materials with both solid and fluid characteristics.</td></tr>
<tr><td>Fluid mechanics
The study of the physics of continuous materials which take the shape of their container.</td><td>Non-Newtonian fluids</td></tr>
<tr><td></td><td>Continuum Thermodynamics
The study of energy conversion</td><td colspan="2">Newtonian fluids</td></tr>
</table>

Conservation equations

Fundamental physical laws such as the conservation of mass, the conservation of momentum, and the conservation of energy are including the physical principles that govern the mechanical response of a continuous medium. These laws allow us to write mathematical relationships of physical quantities like displacements, velocities, temperature, stresses and strains in mechanical systems. The solution to the equations represents the response of the system. The equations of motion and equilibrium e.g. are derived from the fundamental principle of conservation of linear momentum. Heat flow is derived from the energy conservation law.

Constitutive equations

Information about the particular material studied (e.g. material constants) and its response to external agents (e.g. forces or fields) is added through a constitutive relation, expressing that the material is homogeneous or inhomogeneous, isotropic or anisotropic, linear or nonlinear or thermo-elastic or that the material shows plasticity, visco-elasticity, or visco-plasticity. In more general terms the constitutive equations relate the primary field variables (like density, temperature, displacement and velocity) to secondary field variables (energy, heat and stress). The detail employed may be macroscopic or microscopic, depending upon the level necessary to the problem under scrutiny.

These relations might be derived from theory, models at finer scale, experimentally or they might be "phenomenological".
The theoretical derivation of a material's constitutive equations is a common, important, and sometimes difficult task in theoretical materials science. Here, the constitutive equations are determined by calculating how a molecule responds to the local fields. This might e.g. be the Lorentz

force or lattice vibrations in crystals or bond forces. This requires finer scale models like the ones discussed in Chapter 1, 2 and 3.
Phenomenology goes beyond purely empirical data as it involves a certain concept. A phenomenological constitutive equation is not completely based on physical mechanisms responsible for the behaviour. As a rule, phenomenological relations take the form of a system of equations (of algebraic, differential or integral type) with a number of parameters (or functions) to be identified from experiments.

Kinematic constraints

The model equations are the conservation equations. Material information enters the system via constitutive equations and material information can also enter via constraints on the solution. Such constraints are e.g. used in simplified Molecular Dynamics and in Material Mechanics. In Material Mechanics kinematic constraints express the limits on the movement due to the properties of the material.

Geometric changes in a continuous medium (in static or dynamic equilibrium under mechanical and/or thermal forces) are expressed by the conservation laws, constitutive equations and kinematic constraints considered jointly. The solution describes how each little part of a material moves and where it will go and how large a space will be occupied in a certain place and time.
(People involved in continuum mechanics call this solution "the kinematic equations".)

Kinematic behavior as expressed in the solution is often a necessary basis for the formulation of constitutive equations for larger scale models. Also the temperature gradient can be part of this description.

Governing equations

The conservation equations together with the constitutive equations and constraints are called the governing equations.

4.1.1 Solid Mechanics

Solid mechanics is the branch of mechanics, that is concerned with properties and behavior of solid matter under external actions like external forces, temperature changes, applied displacements.

Contact mechanics is the study of deformation and behaviour of bodies that touch each other and may undergo relative motion and contact phenomena such as friction, lubrication, wear, heat transfer.

Modeling of materials behavior under service conditions is about predicting materials behavior under e.g. mechanical (static or dynamic) loading, thermo-mechanical loading, chemically aggressive environment (e.g. all types of corrosion) and combinations thereof.

In continuum modeling also a chain of modeling can be applied that uses the same physics and chemistry equations applied to different scales. When continuum mechanics is applied to the

smaller (nm and µm) scale it is called "continuum micro-mechanics" (note this name refers to the dimensions of the sample only) and the larger scale case is called "macro-mechanics".

Micromechanics

Heterogeneous materials, such as composites, solid foams, poly-crystals and human intervertebral discs, consist of clearly distinguishable constituents (or phases) that show different mechanical and physical material properties. Micromechanics of materials predict the response of the heterogeneous material on the basis of the geometries and properties of the individual phases. The results are then "homogenised" to describe the properties and behaviour of a heterogeneous material. Such properties and behaviour are often difficult to measure experimentally, and micromechanics models can avoid expensive tests that would involve a large number of permutations of constituent material combinations; fibre and particle volume fractions; fibre and particle arrangements and processing histories.

Micromechanics of materials can also evaluate the local (stress and strain) fields in the phases for given macroscopic load states, phase properties, and phase geometries. Such knowledge is especially important in understanding and describing material damage and failure.

Macro-mechanics

The same continuum mechanics governing equations (conservation and constitutive equations of the same form) can be applied to larger (macro) scales and this is called "continuum macro-mechanics". The constitutive equations can either be calculated by micromechanics or experimental or phenomenological constitutive equations can be used.

Examples of micro and macro-mechanics modelling

Heterogeneous materials, such as composites, solid foams and poly-crystals have been modelled a.o. by MATRANS, IMS&CPS and NANOINTERFACE.

CODICE developed micro and macro models to predict the structural evolution of cement.

DISC REGENERATION is modelling the biphasic properties of soft tissues of the intervertebral disc to calculate hydrostatic stresses and deformation of the disc using poro-hyper-elastic constitutive equations.

IMS&CPS is modeling materials consisting of composites or fibers which move during fabrication or during in-service operations.

MODIFY developed a model for the response of polymer acrylics to elongational deformation fields.

NPMIMETIC developed a hybrid model, using the multi body system tool to predict the motion and deformation of intervertebral discs. The kinematics, stress distribution and its effects can be analysed simultaneously, allowing a more precise definition of the loading state of the different parts.

SIMUGLASS is modelling glass behaviour including thermal transport phenomena and large scale deformation in a thermo-moulding process to predict the index drop inside glass material.

Stress-Strain constitutive equations for solid mechanics

A material has a rest shape and its shape departs away from the rest shape due to stress (force per unit area). The amount of departure from rest shape is called deformation; the proportion of deformation to original size is called strain. The strain induces stresses in the material (and vice versa) and how they exactly do this in a particular material is expressed in the constitutive equations for solid mechanics relating the strain to the stress.

There are four major models that describe how a solid responds to an applied stress:

1. Elastically – If the applied stress is sufficiently low (or the imposed strain is small enough), almost all solid materials behave in such a way that the strain is directly proportional to the stress; the coefficient of the proportion is called the modulus of elasticity. This region of deformation is known as the linearly elastic region. When an applied stress is removed, the material returns to its un-deformed state, i.e. no permanent strain remains after unloading. Linearly elastic materials, those that deform proportionally to the applied load, can be described by the linear elasticity constitutive equations such as Hooke's law. When the strain becomes larger the material might react non-linearly and this is called hyper-elasticity.

   DISC REGENERATION is using poro-hyper-elastic constitutive equations in their model for biphasic properties of soft tissues of the intervertebral disc. With this they calculate hydrostatic stresses and deformation of the disc.

   MATRANS is using standard linear thermo-elasticity constitutive equations in their macro-scale thermo-mechanics model. Material parameters in the constitutive equations for composites are obtained from micromechanics.

   SIMUGLASS is using elastic and viscoelastic constitutive equations in their macro-mechanics models and combined with the ideal gas equation they model glass behaviour including thermal transport phenomena and large scale deformation in a thermo-moulding process and to predict the index drop inside glass material.

   SMASH is using linear elasticity constitutive equations in the model for strain in hetero-structures and with this they predict structure parameters for optimised LED performance.

   ROLICER is using elastic and thermo-elastic constitutive equations in ANSYS and ABAQUS to obtain material stresses as a function of material properties and realistic working conditions.

2. Viscoelastically – These are materials that behave elastically, but also have damping: when the stress is applied and removed, work has to be done against the damping effects and is converted in heat within the material resulting in a hysteresis loop in the stress–strain curve. This implies that the material response is time dependent or rate sensitive. This is modeled by constitutive equations resulting from the superposition of the elastic (spring) and viscous (dashpot) models, which can be joined in series (Maxwell solid) or in parallel (Kelvin solid) or as various combinations of spring-dashpot assemblies.

   NPMIMETIC is using an in-house hyper-visco-elastic constitutive equation in their model for bulk material. With this they simulate the mechanical properties of the native nucleus pulposus within the intervertebral disc.

   ROLICER is using an elasto-hydro-dynamics constitutive equation to calculate loading limits.

SIMUGLASS is using elastic and viscoelastic constitutive equations in their macro-mechanics models and combined with the ideal gas equation they model glass behaviour including thermal transport phenomena and large scale deformation in a thermo-moulding process and to predict the index drop inside glass material.

3. Plastically – Materials that behave elastically generally do so when the applied stress is less than a yield value. When the stress is greater than the yield stress, the material behaves plastically and does not return to its previous state. That is, deformation that occurs after yield is permanent. This is modeled by constitutive equations in which the total strain is decomposed into elastic and plastic part. The onset of plastic flow is characterised by a yield condition and the elastic strains are related to the stresses by Hooke's law, whereas the constitutive equation for the plastic strain increment (flow rule) is obtained from the plastic potential, often assumed the same as the yield function. The plastic potential specifies the components (to within a multiplier) and the direction of the vector of plastic strain increment (exterior normal of the flow surface) through the system of partial differential equations.

NANOINTERFACE is using a semi-analytical plasticity constitutive equation for Cu/polymer interfaces to establish cohesive/adhesive interfacial delamination criteria under external loading and to quantify the effect of roughness on adhesive properties.

MATRANS is using elasto-plastic constitutive equations to model residual stresses after sintering of composites and FGMs.

4. Rheologically - Rheology is the study of the flow of ''soft solids' or solids which respond plastically rather than deforming elastically in response to an applied force (see also Chapter 4.1.2). It applies to substances which have a complex molecular structure, such as muds, sludges, suspensions, polymers and other glass formers (e.g. silicates), as well as many foods and additives, bodily fluids (e.g. blood) and other biological materials. This is modeled by constitutive equations of non-Newtonian fluid mechanics or linear or nonlinear viscoelasticity and plasticity.

Here speaking of a linear elastic material, plastic material, viscoelastic material, means that their behavior under external loading follows that of the corresponding constitutive equation.

The above classification does not cover possible non-mechanical effects. Among them, heat conduction and temperature effects play an important role in a number of applications. The next section treats briefly this issue.

Case studies: Governing equations describing behavior of solid materials

Under the action of thermo-mechanical loadings the materials may undergo such processes as fatigue, fracture, creep, wear and oxidation etc. Wear, fatigue and fracture are processes that start at a fine scale and a detailed geometry is necessary to capture these processes otherwise lost in homogenisation. These processes are thus described by a multi-scale approach.

Fatigue/damage

In materials science, fatigue is the progressive and localized structural damage that occurs when a material is subjected to cyclic loading. If the loads are above a certain threshold, microscopic cracks will begin to form. In homogeneous materials, like metals, eventually a crack will reach a critical size,

and the structure will suddenly fracture. In heterogeneous materials fatigue damage can be distributed and material can still bear load notwithstanding excessive micro-cracking.

The shape of the structure will significantly affect the fatigue life; square holes or sharp corners will lead to elevated local stresses where fatigue cracks can initiate. Round holes and smooth transitions or fillets are therefore important to increase the fatigue strength of the structure.

Fatigue is modeled with the solid mechanics equations closed by constitutive damage equations like Miner's, Paris's or Goodman's rule. This system describes how so-called damage variables change under applied stress-strain state and give the change of the load-carrying ability (for example, material stiffness) with the changing damage variables.

For multi-scale modeling at the micro- and macro-scales the same physics (physical principles) for both scales can be used. To model fatigue the energy equations are formulated to describe the energy balance with account for the stress transfer at a fine scale with different possible scenarios of damage localisation. The results are then fed into a macro-scale mechanics model.

IMS &CPS has developed simple in-house solid mechanics analytical & FEM models to describe damage initiation on the macro-scale. The constitutive equation is of the static linear mechanics type. This model predicts transverse damage initiation in carbon fabric/polymer composites with and without carbon nanotubes.

MATRANS is modelling fatigue using the elastic strain energy balance and the particle-matrix interactions. They also use damage theory to model micro-cracking due to residual stresses after sintering. The same physics is used at the micro and macro scale considering the stress transfer between the brittle particles, interphase and ductile-matrix.The constitutive equation is that of linear thermo-elasticity with damage for the ceramic reinforcement and the elasto-plastic for the metal matrix.

RADINTERFACE is using a new hybrid kinetic Monte Carlo-Molecular Dynamics model to describe damage accumulation and with this they generate damage constitutive equations

Fracture mechanics is the field of mechanics concerned with the study of the propagation of cracks in materials. In modern materials science, fracture mechanics is an important tool in improving the mechanical performance of materials and components.

Fracture mechanics is a typical multi-scale problem: the initial crack starts at a very small scale (having a very small process zone). It uses methods of solid mechanics to calculate the driving force on a crack and those of experimental solid mechanics to characterize the material's resistance to fracture. With the knowledge of the crack driving force and the crack resistance Griffith’s or Irwin’s criterion is then used to assess the criticality of a crack.

Macroscopically speaking, the crack propagates if the driving force is larger than the fracture toughness (i.e., Griffith’s energy balance). Now, the driving force and the fracture toughness are both defined by multi-scale processes:

-the driving force is dependent on the mechanics at molecular-meso-micro-macro-scale (i.e., different dissipation mechanisms at different scales such as creation of new surfaces and micro-scale plasticity)
-the fracture toughness is dependent on the physical properties of the material(s) at molecular-meso-micro-macro-scales.

On the macro-scale, the integrity of structural members, such as beams, columns and shafts is also an important issue, which is not only addressed by strength of materials or fracture mechanics methods. The methods employed to predict the response of a structure under loading and its susceptibility to various failure modes may take into account various properties of the materials other than material yield strength and ultimate strength; for example, failure by buckling is dependent on material stiffness and thus Young's Modulus.

CODICE is using constitutive equations in a lattice fracture model in which the continuum is replaced by a lattice beam elements. The constitutive equations are derived from results of a atomistic and analytical micromechanical models calculating the microstructure(linear-brittle behaviour of the phases) which is mapped on the lattice beams by assigning them different properties (elastic modulus and tensile strength of porous cement), depending on where the beams lie (cement grain, inner C-S-H variety, overlapping C-S-H variety).

IMS &CPS has developed simple in-house solid mechanics analytical & FEM models to describe delamination propagation on the macro-scale. This model predicts transverse delamination propagation in carbon fabric/polymer composites with and without carbon nanotubes.

MATRANS is using finite element method to compute configurational forces. The method is capable of treating inhomogeneous (functionally graded) materials under static and dynamic loadings. The crack driving force is computed as function of the loading, the crack length and the elastic properties, which can vary in space. On micro-level a damage mechanics approach was used (i.e. in the thermo-mechnical homogenisation) while in the macro mechanical approach the focus is on fracture mechanical concepts (energy release rate). The damage mechanics approach was rather simple using a maximal principal stress criterion in the brittle ceramics, while a plastic strain criterion was used in the metallic phase. If the damage indicator reached a critical value the element was "killed" from the FEM calculation.

ROLICER is using a solid mechanics model to describe crack nucleation based on traction separation laws. Then they use a macro-scale structural model to study crack formation, crack propagation, and fracture behaviour in ceramic materials. They also examine the fracture properties of silicon nitride. They are testing the assumption of anisotropic fracture of the β-grains with a micromechanical finite elements simulation.

Creep

In materials science, creep is the tendency of a solid material to move slowly or deform permanently under the influence of stresses. It occurs as a result of long term exposure to high levels of stress that are below the yield strength of the material. Creep is more severe in materials that are subjected to heat for long periods, and near melting point. Creep always increases with temperature. Depending on the magnitude of the applied stress and its duration, the deformation may become so large that a component can no longer perform its function. But moderate creep in concrete is sometimes welcomed because it relieves tensile stresses that might otherwise lead to cracking.

The rate of this deformation is a function of the material properties, exposure time, exposure temperature and the applied structural load. Unlike brittle fracture, creep deformation does not occur suddenly upon the application of stress. Instead, strain accumulates as a result of long-term stress. Creep is a "time-dependent" deformation. The constitutive equations for creep are those of the plastic flow (cf. above) with the concept of yield condition and associated flow rule or a creep potential function different than the yield function.

DISC REGENERATION is modeling the effect of creep on the relaxation of soft tissues under sustained compression simulating the standing of a person during daily activities.

Wear

In materials science, wear is erosion or sideways displacement of material from its "derivative" and original position on a solid surface performed by the action of another surface. Wear is related to interactions between surfaces and more specifically the removal and deformation of material on a surface as a result of mechanical action of the opposite surface (see also chemical diffusion under CFD in Chapter 4.1.2)

Impulse wear e.g. can be described by a constitutive equations based on a synthesized average on the energy transport between two travelling solids in opposite converging contact.

The micro-scale calculations are performed to obtain the averaged activation parameter for the oxidation process. The macro-scale calculations are done to explicitly model wear and oxidation. But the time dependent parameters needed to do that are obtained from micro-scale calculation. The temperature distribution around a single asperity can reach very high values. This might be lost in homogenisation as on the macro level, the averaged temperature in the unit cell containing the asperity, can be well below the oxidation threshold. Thus micro scale calculations are needed to obtain the exact temperature distribution around the asperity. To do that standard heat conduction models can be applied with the heat flux acting on the upper surface of the conical asperity. Having this micro-scale temperature, an averaged activation factor for oxidation can be calculated, which allows the oxidation to take place for relatively low temperatures on the macro scale.
In short: on the micro-scale only heat conduction and temperature distribution need to be calculated. But on the micro-level, a completely different geometry is used, a conical asperity, whereas on the macro scale the contact zone could e.g. be flat. On the macro scale other mechanical processes can be simulated, not part of micro-level simulations.

CODICE has developed models for the development of wear and fracture and predicted the degradation by ammonium nitrata of porous cement structures. It is a finite element model, which solves the Nernst-Plank equations over a voxeled cementitious structure (composed of cement grains, C-S-H varieties and pore space) in which ammonium nitrate solutions flow through the porous network. The phenomenological constitutive equations for the wear model import information about the micro-structural changes which take place when the ammonium nitrate ions react with the solid phases and calcium ions are released into the solution. Upon this reaction the diffusion constants are readjusted. The model can simulate the effect of accelerated calcium leaching (an intrinsic osteoporosis-like degradation process) for cementitious structures.

MATRANS is modelling progressive wear. The constitutive equation is of the Archard type, i.e. wear volume is proportional to energy dissipated at the contact interface (equivalently, the wear volume is proportional to normal force and sliding distance). For the description of material deformation, heat transfer, and temperature distribution the same constitutive relation in macro and micro scale are used but calculations are performed assuming different geometries. On the micro-scale the real surface topography is considered, and Finite Element Analysis with thermo-mechanical coupling was used for the calculation of averaged wear-oxidation parameters. In macro scale flat surface was assumed.

Corrosion (oxidation) is to be included in wear phenomena, when the damage is amplified and performed by chemical reactions rather than mechanical action. The constitutive equations can be chemical, but can also be purely phenomenological without any account of the underlying chemical process. In such models the rate of change of mass of the corrosion product (oxide) is related to temperature and time based on experimentally observed relations from thermo-gravimetric analysis (TGA). Chemical properties of the oxide layer are considered through parameters in the phenomenological function approximating results of the TGA.

MATRANS is using a coupled heat conduction model for oxidation and wear to predict oxide masses. On the micro-scale a conical geometry of the asperity is used, whereas on the macro-scale the contact zone is modeled as flat.

New constitutive equations for solid mechanics

Note that the conservation equations are not often subject to new modelling and it is thus rather rare that mechanical models discover new physics. However modelling does take place on the constitutive equations modelling the material properties.

MODIFY developed new macroscopic constitutive equations capable of describing quite reliably the deformation equations (e.g., the shear and elongational behaviour) of the synthesized PSA materials. The new equation utilizes generalized expressions for the strain energy density as a function of the three invariants of the conformation or deformation gradient tensor. In limiting cases, it reduces to known laws widely used to describe hyper-elastic materials, such as the Rivlin-Saunders and Hart-Smith theories.

MULTIHY has developed macroscopic models based on novel set of constitutive equations for H diffusion capable of exploiting the information being derived from the atomistic calculations. The equations are more generalised than those commonly used in the literature, enabling the description of hydrogen diffusion under a broader range of conditions (e.g. temperature variations, trap occupancies) as before.

POCO developed an electro-dynamics constitutive equations relating the polarisability of the CNTs, the electric field applied and the viscosity of the polymer with the torque.

4.1.2 Fluid Mechanics

Fluid mechanics is the study of the motion of fluids due to forces. (Fluids include liquids, gases, and plasmas if sufficiently dense to be a continuum)

The foundational axioms of fluid dynamics are the conservation laws, specifically, conservation of mass, conservation of linear momentum (also known as Newton's Second Law of Motion), and conservation of energy (also known as First Law of Thermodynamics). These can be reworked to give the Navier–Stokes equations, named after Claude-Louis Navier and George Gabriel Stokes, which are a non-linear set of differential equations that describes the flow of a fluid whose stress depends linearly on velocity gradients and pressure. The solution to a fluid dynamics problem typically involves solving these equations calculating speed, pressure, density and temperature.

Flow of electrically conducting fluids (e.g. fluids including plasmas, liquid metals, and salt water) in electromagnetic fields need to be described by coupled Navier-Stokes equations and Maxwell's equations of electromagnetism, which need to be solved simultaneously. This part of fluid dynamics is called magneto-hydrodynamics.

SIMBA is doing plasma modeling for reaction chambers.

Flow models

Modelling efforts simplify the principle physical equations in a number of ways, and set of approximations will be discussed.

Compressible vs incompressible flow

All fluids are compressible to some extent, that is, changes in pressure or temperature will result in changes in density. However, in many situations the changes in pressure and temperature are sufficiently small that the changes in density are negligible. In this case the flow can be modeled as an incompressible flow. Otherwise the more general compressible flow equations must be used. Mathematically, incompressibility is expressed by saying that the density ρ of a fluid parcel does not change as it moves in the flow field.

This additional constraint simplifies the governing equations, especially in the case when the fluid has a uniform density.

Viscous vs inviscid flow

Viscous problems are those in which fluid friction has significant effects on the fluid motion.
The Reynolds number, which is a ratio between inertial and viscous forces, can be used to evaluate whether viscous or inviscid equations are appropriate to the problem.
Stokes flow is flow at very low Reynolds numbers, $Re \ll 1$, such that inertial forces can be neglected compared to viscous forces.
On the contrary, high Reynolds numbers indicate that the inertial forces are more significant than the viscous (friction) forces. Therefore, one may assume the flow to be an inviscid flow, an approximation in which viscosity is neglected completely, compared to inertial terms.
This idea can work fairly well when the Reynolds number is high. However, certain problems such as those involving solid boundaries, may require that the viscosity be included. Viscosity often cannot

be neglected near solid boundaries because the no-slip condition can generate a thin region of large strain rate (known as boundary layer) which enhances the effect of even a small amount of viscosity, and thus generating vorticity. The standard equations of inviscid flow are the Euler equations. Another often used model, especially in computational fluid dynamics, is to use the Euler equations away from the body and the boundary layer equations, which incorporates viscosity, in a region close to the body.
The Euler equations can be integrated along a streamline to get Bernoulli's equation. When the flow is everywhere irrotational and inviscid, Bernoulli's equation can be used throughout the flow field. Such flows are called potential flows.

Laminar vs turbulent flow

Turbulence is flow with a high Reynolds number and is characterized by recirculation, eddies, and apparent randomness. Flow in which turbulence is not exhibited is called laminar. It should be noted, however, that the presence of eddies or recirculation alone does not necessarily indicate turbulent flow—these phenomena may be present in laminar flow as well. Mathematically, turbulent flow is often represented via a Reynolds decomposition, in which the flow is broken down into the sum of an average component and a perturbation component.
Equations for the perturbation component are subject to different models (k-eps, second order models etc).

SIMUGLASS is using an incompressible viscous fluid dynamicsmodel to describe the behaviour of the laminar flow of protection gasses

Newtonian vs non-Newtonian fluids and Rheology

If fluids can be characterized by a single coefficient of viscosity for a specific temperature they are called Newtonian fluids. Although this viscosity will change with temperature, it does not change with the flow rate or strain rate. Only a small group of fluids exhibit such constant viscosity.

For a large class of fluids, the viscosity change with the strain rate (or relative velocity of flow) and are called non-Newtonian fluids. The behaviour of non-Newtonian fluids is described by rheology. These materials include sticky liquids such as latex, honey, and lubricants.

For example, ketchup can have its viscosity reduced by shaking (or other forms of mechanical agitation, where the relative movement of different layers in the material actually causes the reduction in viscosity) but water cannot. Ketchup is a shear thinning material, as an increase in relative velocity caused a reduction in viscosity, while some other non-Newtonian materials show the opposite behaviour: viscosity going up with relative deformation, which is called shear thickening or dilatant materials.

Rheology is the study non Newtonian-fluids or otherwise describes as the flow of matter, primarily in the liquid state, but also as 'soft solids' or solids under conditions in which they respond with plastic flow rather than deforming elastically in response to an applied force. It applies to substances which have a complex molecular structure, such as muds, sludges, suspensions, polymers and other glass formers (e.g. silicates), as well as many foods and additives, bodily fluids (e.g. blood) and other biological materials. Theoretical aspects of rheology are the relation of the flow/deformation behaviour of material and its internal structure (e.g., the orientation and elongation of polymer

molecules), and the flow/deformation behaviour of materials that cannot be described by classical fluid mechanics or elasticity.

MODIFY is studying rheology with the POM-POM tube model to study flow and deformation of acrylic polymers.

MUST is using an in-house diffusion model and phenomenological model of formation of liquid emulsion cores by membrane emulsification (balance of hydrodynamic, capillary and buoyancy forces) to calculate the optimal composition and structure of the coating to deal with corrosion of metallic and polymeric substrates and structures.

ORAMA is using a CFD code for droplet formation and optimization of Ink-Jet and Sol-Gel processes.

Two phase flows

Without the wish to be complete it should be stated that many flows need their own models like e.g. two-phase flows where interactions between the phases have to be modeled.

Constitutive equations for flows

Besides modeling of the fundamental physics equations, there are also different constitutive equations in use and some projects have developed new ones.

Fick's law

Fick's first law relates the diffusive flux to the concentration under the assumption of steady state. It postulates that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient (spatial derivative). This constitutive equation is used to close the conservation of mass (flow) equations reduced to diffusion only.

Constitutive equation for the diffusion of chemical species

Diffusion of interstitial atoms due to chemical potential gradients can be described by an extended Fick's diffusion equation with added terms due to chemical potential gradients (stress and temperature).The Nernst–Planck equation is a constitutive equation used to close the conservation of mass equations to describe the diffusion of charged chemical species in a fluid in an electric field. It relates the flux of ions under the influence of both an ionic concentration gradient and an electric field. It extends Fick's law of diffusion for the case where the diffusing particles are also moved with respect to the fluid by electrostatic forces. If the diffusing particles are themselves charged they influence the electric field on moving. Hence the Nernst–Planck equation is applied in describing the ion-exchange kinetics. Please see also the diffusion equation described at atomistic level.

ARTIVASC used a constitutive equation of the Nernst-Planck type in the advection-diffusion-deposition model for the permeation-times of nutrients and O2.

MULTIHY is using Fick's diffusion equation as constitutive equation extended with terms due to chemical potential gradient and trapping. This is used with codes to obtain a description of hydrogen diffusion under broader range of conditions (temperature variations, trap occupancy) at the specimen and component level.

CODICE used the Nernst-Planck constitutive equations simulating grain-based flow and hydrogen diffusion with their continuum model.

Poro-elastic flow

When fluids are streaming through a porous medium a combination of solid mechanics and fluid mechanics is to be applied. Two mechanisms play a key role in this interaction (i) an increase of pore pressure induces a dilation of the porous solid, and (ii) compression of the solid causes a rise of pore pressure, if the fluid is prevented from escaping the pore network.

The fluid transport in the interstitial space can be described by the well-known Darcy's law, which is an empirical (phenomenologically) derived constitutive equation that describes the flow of a fluid through a porous medium (see also Chapter 4.1 flow). Darcy's law works with variables averaged over several pore-widths. It can also be derived from Navier-Stokes equations by dropping the inertial terms, so this is an example of a constitutive equation being derived from the physics equations. Darcy's law is a simple proportional relationship between the instantaneous discharge rate through a porous medium, the viscosity of the fluid and the pressure drop over a given distance.

DISC REGENERATION coupled poro-hyper-elastic constitutive equations and vascular transport models to predict the movement of solutes within the intervertebral disc. They simulated the disc mechanical response to external compressive loads which affect diffusion of oxygen and lactate and thus their content within the disc. They also simulated fluid-solid interaction within high porous polymer implants as well as interaction between implants itself and surrounding intact biological structures and test different disc replacement configurations.

Scales

Also in this part of continuum mechanics models can be created for the behaviour at different scales and also in this discipline a chain of flow models at different scales might be used.

State-of-the-art models for flow at the smallest scale are e.g. the so called "atomistic" finite elements which can be applied to length scales of 100 nm – mm and timescale of ms to s. (This scale is called meso by electronic modellers and micro by continuum modelers, here the first name is adopted.)

The calculated properties can be used as constitutive equations in the flow models at higher scales.

4.2 Continuum thermodynamics (including heat transport)

A part of continuum mechanics is called thermodynamics and deals with the conversion of energy (hot engines, cooling systems, etc.). Thermodynamics is also used in the modeling of materials.
The first law of thermodynamics states, that energy is conserved.
The energy related to the atomic and molecular structure of the material and the degree of their activity is independent of outside reference frames and is called internal energy. The macroscopic energy is the kinetic energy and potential energy of the material sample. The only two forms of energy interactions are heat transfer and work. The second law relates kinetic energy and internal energy to the power exerted on/by the system and the heat transfer.

For each application it has to be decided which forms of energy have to be taken into account in the model. The portion of the internal energy associated with the kinetic energies of the atoms/molecules (rotation and vibration of the atoms about the center of mass) is called sensible energy. The internal energy associated with the atomic bonds in a molecule is called chemical energy. Mutual potential energy of the atoms as they change their distance inside the molecules is part of the internal energy. Stresses in the material can be regarded as part of the internal energy. The energy associated with the phase –change process related to the binding between molecules is called latent heat. Nuclear energy is not considered in NMP projects.

> *Internal energy and temperature*
> *Temperature is a measure of the average kinetic energy of the center-of-mass motion of individual molecules. In daily life sensible and latent energy are called "heat", while in thermodynamics it is called thermal energy to distinguish it from heat transfer.*
> *Energy can be put into a material in many ways (friction, radiation, conduction, kinetic impacts etc.). Some part of the energy goes into vibrations and rotations about the center of mass (if not a mono-atomic gas) and only a part of it ends up as increasing the temperature.*

The second law is often considered to fall outside the domain of continuum mechanics. This additional law determines the direction into which this energy flows via the concept entropy.
All mechanical energy can be changed into internal energy, but one can change only a fraction of the internal energy into work.

IMS -CPS does thermodynamics models of percolation at nm scale to predict percolation thresholds of composites.
MONAMI does continuous thermo-dynamical and kinetic modelling of local mass density and energy density.

Thermo-mechanical behaviour

Thermomechanics studies the properties of materials as they change with temperature. The materials might show a change of dimension (expressed in the calculated macroscopic thermal expansion coefficients) or of a mechanical property. The bonding in the material determines this response. Crystallinity and fillers introduce physical constraints to motion. Cross-linking between molecules will restrict the molecular response to temperature change since the degree of freedom for segmental motions is reduced as molecules become irreversibly linked.

<u>Principle physical equation describing heat flow</u>
The conservation of energy equation contains the energy change due to heat flow. This term can be modeled by different assumptions and this is expressed in different constitutive equations.
Heat transfer may take place due to conduction (also called diffusion), convection (energy taken away by the surroundings solids or fluids) or radiation.

<u>Constitutive equations</u>
The thermo-elastic constitutive equation defines a relationship between stress, strain and temperature, and thermal conductivity equation relates the heat flux density to temperature gradient. For anisotropic solids, both have to be written in a tensor form. Coefficients of these

equations depend themselves of the temperature and represent thus material functions rather than constant parameters for a specified material. Other material functions determine temperature dependence of parameters in constitutive equations of plasticity, visco-plasticity and rheology. Such material functions are usually determined empirically.
A constitutive equation for conductive heat flow is the Fourier's law that states that the heat flow is proportional to the temperature gradient.
A constitutive equation for convective heat flow can be Newton's law of cooling.
A constitutive equation for radiative heat flow is the Stefan Boltmann's law.

MATRANS modelled the effective linear thermo-elastic properties of the functionally graded materials with micromechanical (incl. heat conduction) approaches and the optimal content of the ceramic phase was searched for meeting the required thermo-mechanical properties of the composite for the target applications.
A multi-scale model of thermal residual stresses in graded metal-ceramic composites, generated during the cooling phase of the sintering process, was developed. The constitutive equations used in the finite element computations of thermal stresses were those of linear elasticity for the ceramic and elasto-plasticity for the metal phase.
MATRANS is using parameters of thermal conductivity and thermal expansion as well as mechanical properties at elevated temperatures to characterize quality of composite materials.

Phase field models are constructed in order to reproduce a given interfacial dynamics. For instance, in solidification problems the front dynamics is given by a diffusion equation for either concentration or temperature in the bulk and some boundary conditions at the interface (a local equilibrium condition and a conservation law) which constitutes the sharp interface model. A number of formulations of the phase field model are based on a free energy functional depending on an order parameter (the phase field) and a diffusive field (variational formulations). Equations of the model are then obtained by using general relations of Statistical Physics. Such a functional is constructed from physical considerations, but contains a parameter or combination of parameters related to the interface width. Parameters of the model are then chosen by studying the limit of the model with this width going to zero, in such a way that one can identify this limit with the intended sharp interface model.

HIPERSOL does phase field modelling of diffusion and firing with COMSOL to calculate the dissolution and transport of Ag.

MINTWELD is using phase field models (nm and µm scale) to describe grain boundary and interface chemistry and structure.

4.2 Chemistry and reaction kinetic models (meso and macro)

Chemical kinetics models are mathematical models that describe the characteristics of a chemical reaction. Normally, all the different chemical intermediate molecular species are represented explicitly. These models are based on thermodynamics and the law of mass action, which states that the speed of a chemical reaction is proportional to the quantity of the reacting substances.

Although some of the parameters in the kinetic reaction models need to be determined experimentally, such models can still be re-used for a wide range of operating conditions and are more versatile than purely empirical phenomenological methods ("operational" kinetics).
Chemical kinetics models are used to determine the rates of chemical processes and how different experimental conditions (e.g. the physical state of the reactants, the concentrations of the reactants, the temperature at which the reaction occurs, and whether or not any catalysts are present in the reaction) can influence the speed of a chemical reaction. They yield information about the reaction's mechanism and transition states and can be used in combination with other continuum models to take into account the changing relative concentration of the chemical species.

FREECATS is using a reaction kinetic model combined with hydrodynamics at nm scale to detail surface reactions and adsorption processes of the new catalysts.

NANOINTERFACE is using an exponential continuum cohesive-zone model to quantify metal-oxide-polymer adhesion properties at the macro-scale level.

NEXT-GEN-CAT is using catalytic reaction kinetic models (CO oxidation, CxHy oxidation and NOx reduction) for the simulation of species concentration in gas near and far from catalytic surfaces along the flow direction.

SUPERLION is doing electrochemical modelling to simulate current-voltage relationships for the porous electrodes.

4.3 Electromagnetism (optics, magnetics, electrical)

Electromagnetism is the branch of science concerned with the forces that occur between electrically charged particles. In electromagnetic theory these forces are explained using electromagnetic fields. Electromagnetic force is one of the four fundamental interactions in nature, the other three being the strong interaction, the weak interaction and gravitation.

The electromagnetic force is the one responsible for practically all the phenomena one encounters in daily life above the nuclear scale, with the exception of gravity. Roughly speaking, all the forces involved in interactions between atoms can be explained by the electromagnetic force acting on the electrically charged atomic nuclei and electrons inside and around the atoms, together with how these particles carry momentum by their movement. This includes the forces experienced in "pushing" or "pulling" ordinary material objects, which come from the intermolecular forces between the individual molecules in our bodies and those in the objects. It also includes all forms of chemical phenomena.

In classical electromagnetism, the electromagnetic field obeys a set of equations known as Maxwell's equations, and the electromagnetic force is given by the Lorentz force law.

The dynamics of free charges and currents are described by Maxwell's equations directly, but the dynamics of bound charges and currents enter Maxwell's equations through the constitutive relations.

The constitutive equations link the electrical and magnetic field to the electrical flux density (displacement) and the magnetic flux density. Each type of material (magnets, conductors etc) has their own relation.

The projects AMON-RA used the Maxwell equations and semi-classical drift-diffusion model for the calculation of optical properties.

MAGNONICS makes electromagnetic and spin dynamics models using the dynamical matrix method and Ewald-FFT method to calculate the magnetic behaviour of dipole-coupled and arrays of anti-dots and the magneto-dipole interaction field, to characterise the nature and spatial structure of magnons in magnonics array

METACHEM uses the Maxwell equations (nm scale) and generalised Mie model (mm scale) to calculate individual polarizabilities of complex scatterer (electric and magnetic), surface susceptibilites of metasurfaces (electric, magnetic and magnetoelectric), refractive index, thickness and bi-anisotropy of metamaterials and to calculate scattering by cluster of simple and core-shell spheres in order to determine optical devices performance with metamaterials

MONAMI used a coarse grained model with effective soft potentials for calculation of spin dynamics in small magnetic clusters

NIM-NIL did characterisation based on electromagnetic wave theory (Maxwell solver) to describe the dissipative loss in resonant electromagnetic metamaterials. The model takes into account the radiation damping of the resonant currents.

POCO developed electro-dynamics constitutive equations for the alignment of CNT under electric fields. They used these to describe crystallisation of thermoplastics with and without CNT and for the determination of alignment of CNT in viscous media under electric fields.

SMASH uses electromagnetic models for the calculation of optical properties of nanorods, optical extraction efficiency, emission directionality and polarization and to calculate the radiation characteristics as input to processing technologies

Magnetics, Elect(ron)ics and Optics.

Electromagnetics at electronic level is discussed in Chapter 1

The continuum level is not discussed here and the reader is referred to the literature. It is only noted that electric fields and magnetic fields are different aspects of electromagnetism, and hence are intrinsically related. A changing electric field generates a magnetic field and via versa.

AMON-RA calculates the electrical properties of nanowire arrays of the Esaki interband tunneling diode and electronic transport simulation in large diameter hetero-junction nanowires with tunnel junctions.

IMS&CPS models electrical conductivity and percolation at nm scale to predict electrical conductivity and percolation thresholds of composites

IRONSEA models resistively and capacitively shunted junctions with electrical device modelling to calculate the characteristic of junctions based on Fe-based superconducting films.

MINOTOR uses classical micro-electrostatic model (at nm scale) to calculate energetic profile of the charge carriers around the interface to optimize mechanism of chemical doping in organic layers providing energetic disorder

Optics is the branch of physics which involves the behaviour and properties of light, including its interactions with matter. Because light is an electromagnetic wave, most optical phenomena can be accounted for using the classical electromagnetic description of light.
Some phenomena depend on the fact that light has both wave-like and particle-like properties. Explanation of these effects requires quantum mechanics and this is discussed in Chapter 1.

ORAMA uses electromagnetic codes to calculate magnetic and optical properties of their devices.

Chapter 5
Process and Device Modelling

Once the material has been designed it has to be produced. The manufacturing processes too can be designed and optimised via modelling. And, last but not least, the material will be used in applications and integrated in devices, and also this can be optimised via modelling.

MORDRED uses RANDOMSPICE to predict reliability of electronic devices. RANDOM SPICE is a Monte Carlo circuit simulation engine for ICT devices, which enables simulations of statistical and process variability, data harvesting and statistical analysis of the simulation results. RandomSpice provides the facilities necessary for accurate statistical circuit and standard cell characterisation, and supports power–performance–yield (PPY) analysis. Input includes bias, temperature, materials etc., but also a lot of non-physical fitting parameters, and output is current/voltage behaviour.

NEXT-GEN-CAT is doing process modelling with mass, energy and momentum balances to predict the performance of catalytic converters and to predict the concentration distribution of the chemical species.

ORAMA is doing PVD and process control for deposition in a PVD chamber.

SIMBA is using FLUENT with CFD models for plasma incl EM, thermodynamics and chemistry processes to calculate the behaviour of a lab-scale reactor including non-equilibrium plasma and nanopowder nucleation out of the gas phase.

SUPER-LION is doing nano-scale battery architecture models with MCGEN and DL-POLY to calculate the efficiency of the battery.

Chapter 6
Linking of models and Numerics

6.1 Linking different models (multi-scaling and multi-modelling)

Depending on the timescale of the phenomena and the accuracy needed, models at different time- and length-scales can be applied and the results need to be transferred from one model to another. This is here called multi-scale modelling.

It might also happen that different physics and chemistry need to be coupled at the same scale like solid and fluid mechanics with thermodynamics or reaction kinetics. This is called here multi-modelling as the models are applied to the same length- and time- scales and the word multi-scaling does not really apply.

Developing composites for aircraft is a multiscale problem, where first the fiber-matrix system is modelled at electronic and atomistic level, then the composite ply at mesoscale level, and finally the laminate and structural part for the airplane at macroscale level. (IMS&CSP)

Problems may be multi-physics like the study of hydrogen embrittlement of materials and components. The processes to be described are hydrogen diffusion, then chemical reaction then viscoelastic behaviour (MULTIHY).

The multi-scale framework developed in NANOINTERFACE starts with Molecular Dynamics simulations to describe the thermo-mechanical and failure behaviour of epoxies, copper, copper oxides and the respective interfaces. At the meso-scopic level, coarse grained models are used to transfer structural and force information from molecular simulations to continuum and vice versa. At the continuum scale, metal-oxide-polymer adhesion properties are determined by describing the relevant dissipative mechanisms that affect adhesion, including the underlying microstructural mechanisms obtained through a sequential coupling.

The project NEXT_GEN_CAT calculated reaction kinetics of catalysts reactivity with ab initio modelling. This will be used in fluis flow simulations for the prediction automotive catalytic converter performance.

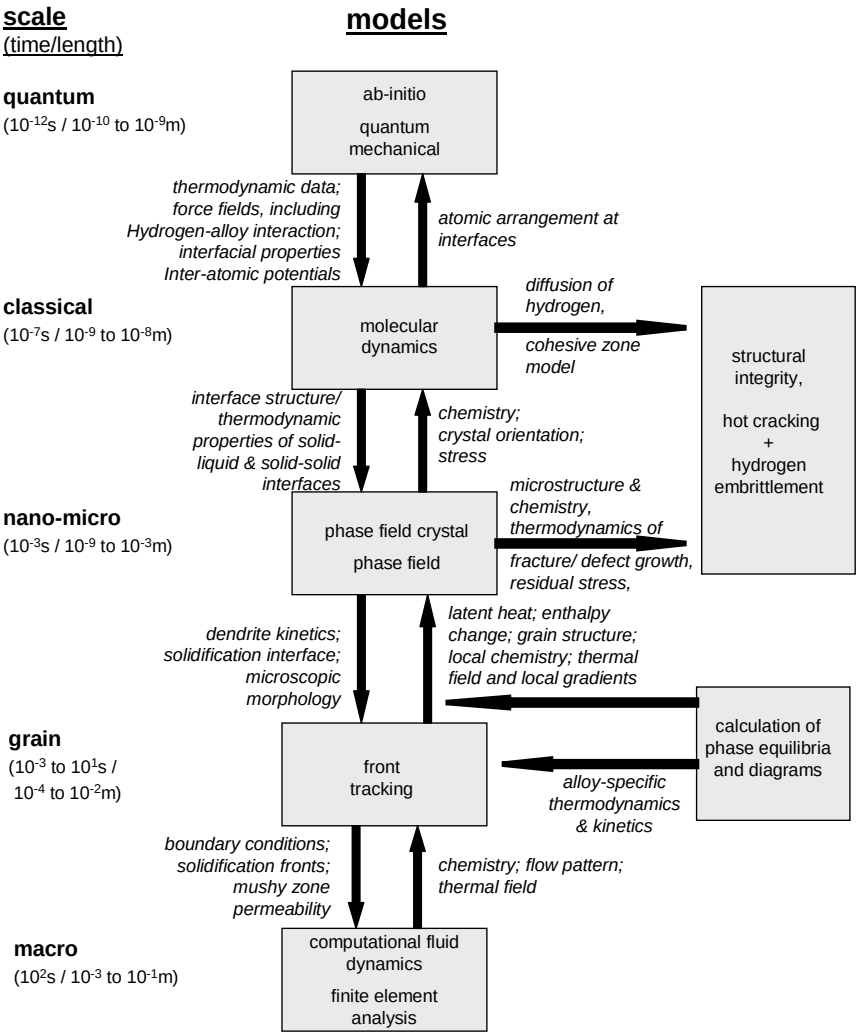

Fig 1. Data flow in multiscale modelling in MINTWELD (Hongbiao Dong, Leicester University, UK)

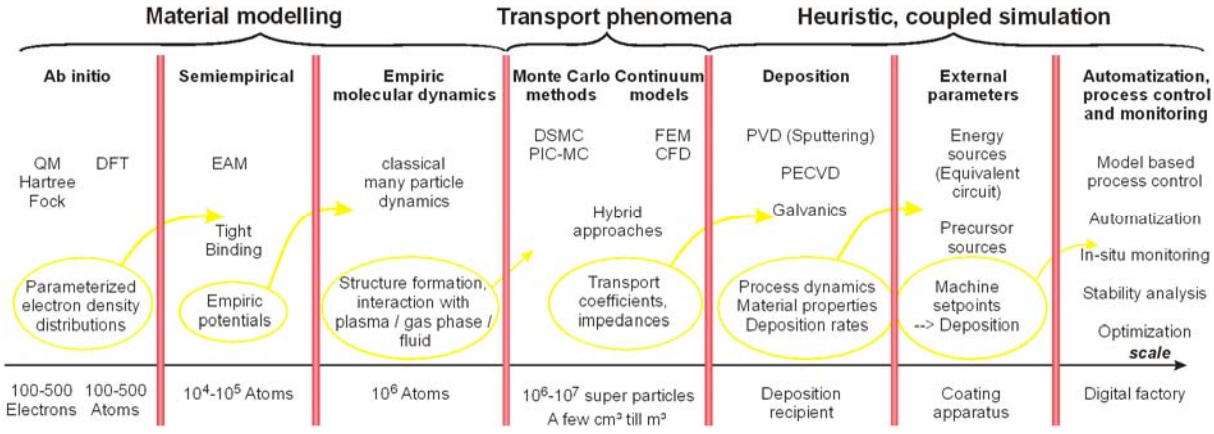

Fig.2 Data flow in multi-modelling linking in ORAMA (Bernd Szyszka, FhG, DE)

6.1.1 Linking between different electronic models

In IRON-SEA modelling is used to calculate transport properties in superconductors (mainly Josephson Junctions). The multiband Eliashberg model requires input from band structure calculations (normal DOSs at the Fermi levels) provided by the Blonder-Tinkham-Klapwijk model.

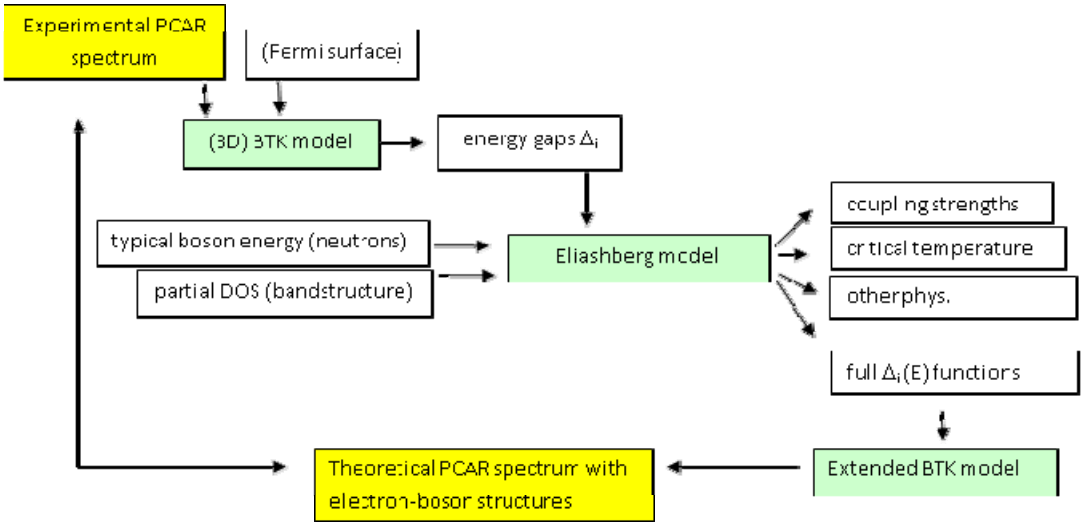

Fig 3 Linking of electronic models in IRON-SEA (Kazumasa Iida, Institute for Metalic Materials, DE)

6.1.2 Linking of electronic and atomistic models

ATHENA combines electronic structure calculations at the level of DFT with model Hamiltonian schemes for simulating the thermodynamical properties of complex oxides and oxides interfaces. The electronic structure is then mapped onto model Hamiltonian via the rigorous Wannier function scheme. Then the model Hamiltonian is solved at the Monte Carlo level for extracting finite temperature properties of oxides and their interfaces. These properties include magnetic order, critical temperature for magnetism, conductivity, ferroelectric distortion.

FEMTOSPIN uses ab-initio information (spin, exchange integrals, anisotropy) to parameterise atomistic and heat bath model calculations. A multiband Hubbard model is under development and will be used to improve the calculation of the exchange field in disordered systems and the introduction of longitudinal spin fluctuations

HIPERSOL is connecting DFT and molecular dynamics with a finite element model of the current transport from the silver finger to the silicon in a standard Si-based solar cell. The interfacial resistivities are obtained from Schottky barriers calculated with DFT based on atomic interface models optimised using empirical molecular dynamics.

The MONAMI project has done simulations of magnetisation dynamics. First the electronic structure is modelled with density functional theory and this is used as input for atomistic length-scale models for spin-dynamics.

MUST uses the ab-initio quantum chemical calculation to determine some of the force field parameters for the molecular dynamic simulations of adsorption of polyelectrolytes during the layer-by-layer formation of thin film coatings and capsule shells.

NAMASTE has performed density-functional and microscopic tight-binding Anderson calculations of the band structure of ferromagnetic semiconductors. Results of these calculations served as a justification for the choice of an effective Kondo spin Hamiltonian and provided the values of the Kondo Hamiltonian parameters. The effective model Hamiltonian description served then as a basis for calculating a wide range of thermodynamic magnetic properties and magneto-transport properties with a special focus on spin-orbit coupling induced effects.

ORAMA used parametrised electron density distribution obtained through ab initio quantum mechanical models to develop semi-empirical potentials. These were used in molecular dynamics simulation at the atomistic scale.

OXIDES is interfacing electronic and atomistic calculations through DFT calculations which will set the basis for the derivation of the appropriate effective Hamiltonians describing how the ferro-electric and anti-ferroelectric domain distortions couple to each other at the interface and what the relevant an-harmonic interactions are. The effective Hamiltonian should be able to capture the physical effects which dominate the behaviour of super-lattices.

SMASH is using amulti-scale model where atomistic band structure calculation on a sub region is linked to a continuum drift-diffusion type electronic transport model.

6.1.3 Linking between electronic and continuum models

AMON-R uses a multi-physics model where electromagnetics are coupled to drift diffusion continuum models.

IMS&CPS has developed electrical models of carbon nanotubes at nano-scale to study electron displacements between nanotubes. In parallel, macro-scale models of solid continuum mechanics are performed to predict the mechanical behaviour of a composite part (a landing gear door of civil aircraft). When the optimal location of nanotubes in the composite is determined at nano-scale, the mechanic model at macro-scale is modified to add the carbon nanotubes in the analysis of the mechanical behaviour of the composite part.

NEXT_GEN_CAT aims at linking DFT calculations with full scale catalytic converters simulation. Adsorption energies and reaction barriers obtained through DFT methods provide the basis to develop a surface reaction mechanism. This has to be included in continuum models of the non-isothermal, reacting flow bounded by catalytic surfaces, to simulate experimental activity measurements of different PGM-free catalysts

SMASH used a multi-physics model where linear elasticity theory is coupled to electronic band structure calculation which itself is coupled to a drift-diffusion system. Within the drift-diffusion electron transport system, a k.p-method is coupled to take care of the regions where quantisation processes of carriers take place. The result of this model is then taken as input to calculate the electromagnetic problem for the extraction efficiency.

6.1.4 Linking between different atomistic models

MINTWELD carried out ab-initio simulations molecular dynamics calculations to predict multi-component force fields and to provide an extensive configurational database for the energetics and dynamics of alloys in complex environments. These data will be used as input in Molecular dynamics modelling. Molecular dynamics modelling was then performed to explore the process of grain boundary formation under various conditions using results from micro-scale phase-field modelling as input data. The atomic-scale grain boundary structure and chemistry will be determined and this information will then be used in Ab-initio simulations and micro-scale phase-field modelling

6.1.5 Linking of atomistic and mesocale models

CODICE used atomistic simulations to identify the smallest bricks of cementious structures. By employing Molecular Dynamic simulations CODICE has revealed that the main constituent of cement hydration (C-S-H) is nano-branched, with segmental pieces of 3x3x6 nm-sized. Afterwards, these segmental pieces have been approximated by 4-5 nm-sized spherical particles which served as coarse grained particles in a home-made Kinetic Monte Carlo scheme. This KMC scheme has enabled to describe larger structures of C-S-H gel and establish a linkage with a new continuous chemical model which provide microstructural information .

DYNAMAG and MAGNONICS used ab-initio calculations are used to calculate the saturation magnetisation, the exchange stiffness and the anisotropy constants of magnetic materials and the strength of the exchange interaction and surface anisotropy at interfaces in composite magnetic materials. The parameters are then used in micro-magnetic simulations e.g. on the basis of the Landau-Lifshitz equations.

FEMTOSPIN used atomistic models are used to calculate temperature dependence of magnetisation, anisotropy and longitudinal and transverse susceptibilities for use by mesoscopic (micro-magnetic) models

In MINOTOR, outputs from quantum-chemical calculations were fed into micro-electrostatic models to determine the energy landscape of the charge transport levels in molecularly doped organic semiconductors. Realistic morphologies have been obtained with Molecular Dynamics simulations based on force fields. The electronic coupling (transfer integral) between the molecules has been computed on that basis with quantum-chemistry (DFT) approaches. The distribution of site energies (HOMO/LUMO levels) has also been calculated with the help of a self-consistent microelectrostatic (classical) approach parameterized with the help of quantum-chemical calculations. The motion (and hence the mobility) of the charges has been estimated by evaluating transfer rates on the basis of the calculated molecular parameters and by plugging them into Kinetic Monte Carlo simulations.

MORDRED used first principles simulations describing the atomic and electronic structure of the sources of fluctuations (discrete dopants, localised defects, interface roughness, body thickness, composition, strain, structure variation) in oxide interfaces to parameterise hierarchical device simulations in order to predict realistically intrinsic fluctuations in CMOS devices.

NAMASTE used some of the results of the atomistic calculations, including the magnetization, magnetic anisotropy constants, spin stiffness, and Gilbert damping parameter as inputs into the phenomenological Landau-Lifshitz-Gilbert micro-magnetic simulations of various magnetization dynamics phenomena of relevance to the devices studied in the project.

ONE-P modelled the charge mobility in the bulk of organic semiconductors. On the basis of a generated morphology, first the rate of charge hopping between two molecules is computed by evaluating at the quantum-chemical level the relevant parameters (transfer integral, reorganization energy, energetic disorder). In a next step, the rates are injected into Kinetic Monte Carlo simulations to propagate the charge carrier(s) and estimate the mobility from the total distance travelled during the time of the simulation.

In ORAMA the multifunctional oxides structures resulting from molecular dynamics simulations at the atomistic scale have been fed into mesoscale models that solve the Boltzmann transport equation for the description of gas flow phenomena by means of Direct Simulation Monte-Carlo (DSMC) techniques. With self-consistent electric field computation that approach is extended to Particle-in-Cell Monte-Carlo Techniques (PIC-MC) for plasma phenomena.

6.1.6 Linking of atomistic models and continuum mechanics

HIPERSOL has calculated diffusivities of Ag and other elements in different silver pastes (glasses) with first principles molecular dynamics and used this as input to a phase-field model (with Gibbs free energies taken from a thermodynamic database) of transport of silver through a glass layer.

In MINTWELD micro-scale Phase Field modelling is used obtain a complete picture of microstructure and defect (e.g. cracking) formation in the welding process, as illustrated in Fig 1. Atomistic molecular dynamics simulations provides the structure of the interface and its thermodynamics properties as input. The predicted results on transformation kinetics and interface morphology is fed to grain-scale models; the calculated chemistry and crystal orientation and stress can be used as input for molecular dynamics modelling.

MODIFY developed a macro-scale model for the response of polymer acrylics to elongational deformation fields. This model relies on information from a atomistic model for molecular structural changes upon stretching, which computes the entanglement network.

MULTIHY will employ novel constitutive equations for hydrogen diffusion and trapping that are informed by atomistic descriptions of the occupancy of different trap sites with respect to lattice concentration and their effect on the overall diffusion rate, there by enabling use of atomistic results at the continuum level.

MUST used molecular mechanics for modelling of the limiting adsorption of organic anticorrosive or hydrophobizing agents. This information is then used as the boundary condition for the transport(diffusion) equation to determine the critical concentration of agents in capsules and of capsules in multifunctional coating necessary to achieve protection of the damaged surface. Similar methodology was used to predict surface activity (i.e. determine the hydrophilic-hydrophobic ratio) of selected compounds with silanol groups, which can be used to built the silica shell around the capsule core. In addition the MD simulation of the L-b-L formation of polyelectrolyte shells allow

determination of its porosity, which enters as a parameter for prediction of the release rate of anticorrosives from capsules.

The multi-scale framework developed in NANOINTERFACE starts with Molecular Dynamics simulations to describe the thermo-mechanical and failure behaviour of epoxies, copper, copper oxides and the respective interfaces at the atomic scale. At the mesoscopic level, coarse grained models are used to transfer structural (thermo-mechanical and failure) information from molecular simulations to continuum scale. At the continuum scale, metal-oxide-polymer adhesion properties are determined by describing the relevant dissipative mechanisms that affect adhesion, including the underlying microstructural mechanisms obtained from the mesoscopic scale through a sequential coupling.

NANOMODEL linked MolecularDynamics and ContinuumMechanics models. They are closely connected, via forward and reverse mapping schemes.

6.1.7 Linking of mesoscale and continuum mechanics

In MINTWELD macro-scale CFD modelling is taking into account a wide range of predicted thermal and grain structure information of welded interfaces to relate the process variables to the properties of the weld pool. The dynamics of welding interface evolution is being solved to give the local chemistry and the flow of molten liquid in the weld pool, through linking the macro-scale models with the meso-scale solidification model. Grain scale (Meso-scale, from cm to tens of μm) models are being used to model grain structure evolution, such as grain size and distribution, and local solidification profile (e.g. mushy zone) for macro-scale computational fluid dynamics (CFD) modelling of weld flow; predicted thermal and grain structure information is used as input for micro-scale continuum modelling, as shown in Figure 1.

MUST uses the DPD modelling in parallel with the continuum modelling of transport of anticorrosive or protective agents in the cracked coatings to determine the values of effective parameters used in continuum approach. The solution of diffusion equation in inhomogeneous media, based on the lattice gas model and finite differences were elaborated. Finally the one dimensional diffusion equation describing water (or ions transport) in the effective medium was derived using the values of the effective parameters devised basing on the discrete 2D and 3D approach. In the model various triggering mechanisms of the release of inhibitor from containers as concentration thresholds of corrosive ions or corrosion products were considered. Single and multilayer coatings were simulated with the arbitrary distribution of water, ion traps and inhibitor containers.

6.1.8 Interchange between different continuum models

Within DYNAMAG and MAGNONICS, micro-magnetic simulations are run to determine magnetic response of nanostructured materials (mainly resulting from magnonic responses). The output is used to calculate magnetic susceptibility of the magnonic meta-atoms. Using appropriate homogenisation procedures, the susceptibility is then used to calculate the magnetic permeability of corresponding magnonic metamaterials, which is then used with Maxwell equations to explore how electromagnetic waves propagate in such metamaterials.

METACHEM is linking the response of structured media with equivalent parameters of homogeneous media. They link equivalent permittivity representations at bulk material level

with full-wave continuous-domain simulations. Those in turn are linked with equivalent-parameter representations for structured media.

MUST uses the large scale modelling of transport of anticorrosive or hydrophobizing agent to the damaged area in the protective coating together with statistical analysis to determine probability of achieving satisfactory corrosion protection at a given concentrations of capsules and agents in capsules (i.e. the technical risk analysis of "not performing").

NANOINTERFACE is linking solid mechanics with chemistry models to describe the thermo-mechanical and failure behaviour of epoxies, copper, copper oxides, and the respective interfaces. The data transfer mechanism involves thermo-mechanical and failure properties by means of sequential coupling.

NEXT-GEN-CAT is coupling fluid flow characteristics of exhaust gases within a real catalytic converter with the equations derived from the mass and energy balances.

6.1.9 Combination of flow models with thermomechanics

DISC REGENERATION coupled mechanical deformation of the disc with diffusion and convection of small solutes within the disc and vertebra.

FREECATS used a CFD code with kinetic equation results as boundary conditions and micro-model for heat conduction (mm scale) to resolve macroscopic heat, mass, momentum transport in boundary layers near catalytic surfaces.

6.2 Numerics

In the fiches (Annex 1) hints are given of the specific numerical features of the simulations done. We would like to highlight a few of them., but for the details the reader is referred to the specialised literature.

Discretisation methods are used to allow numerical solving of the governing equations and these include

- Finite difference methods
- Finite volume methods
- Finite element methods or analysis (FEM or FEA)
- Spectral element methods
- Boundary element methods

In all of these approaches the same basic procedure is followed:

1. During preprocessing
    a. The geometry (physical bounds) of the problem is defined.
    b. The volume occupied by the material sample is divided into discrete points or cells (the mesh). The mesh may be uniform or non uniform.
    c. The physical modeling is defined – for example, the equations of motions + enthalpy + radiation + species conservation
    d. Boundary conditions are defined. This involves specifying the fluid behaviour and properties at the boundaries of the problem. For transient problems, the initial conditions are also defined.
2. The simulation is started and the equations are solved iteratively to converge to as a steady-state or to describe transient situations.
3. Finally a postprocessor is used for the analysis and visualisation of the resulting solution. Extraction of data for further model can be done.

CODICE developed a novel digitalization model that generates a 3D voxel structure of the virtual microstructure and can be used for information exchange within the run of each time step. This new model employs as input macroscopical processing variables, such as the cement grain size, the water/cement ratio, etc. and gives for each voxel relevant information like density, relative humidity, saturation, chemistry, etc.

MODIFY developed a powerful finite-element code for the full three-dimensional (3-d) simulation of the deformation of acrylic adhesives. It is based on a consistent coupling of an elliptic-mesh generation methodology with domain decomposition and local mesh refinement around deforming and moving interfaces. The transport code can follow the large adhesive and bubble deformations inside the material (which lead to fibrillation); it can also trace the elastic boundary layers that form at the moving interfaces. It can therefore reliably simulate the force-deformation history of the material under industrially relevant conditions.

NANOINTERFACE has obtained interchange between Molecular Dynamics and continuum mechanics by creating a finite element "boundary" around the Molecular Dynamics boxes and defining so-called "anchor atoms" reaching into the "boundary". The anchor atoms are part of the polymer chains within the MD domain. In the continuum domain, they are coupled to the finite elements and moved along with their displacements.

NANOMODEL has developed numerical techniques for Molecular Dynamics models to do a coarse graining of the nanocomposite . they then-impose stochastic boundary conditions with a dissipative particle dynamics thermostat on the grains. I information on forces and positions is then transfreed via fixed anchor points.

Smoothed-particle hydrodynamic (SPH) calculations are a computational method used for simulating fluid flows. The smoothed-particle hydrodynamics (SPH) method works by dividing the fluid into a set of discrete elements, referred to as particles. These particles have a spatial distance (known as the "smoothing length"), over which their properties are "smoothed" by a *kernel function*. It is a mesh-free Lagrangian method (where the coordinates move with the fluid), and the resolution of the method can easily be adjusted with respect to variables such as the density.

Smoothed-particle hydrodynamic model has been used to predict wall shear stresses at the vascular graft walls (ARTIVASC_3D).

Accelerated simulations in molecular dynamics

The main problem of standard molecular dynamics is that the time of the simulation sampling is often not long enough to ensure the ergodic theorem can be applied. For example, "centuries" on their available supercomputer would be needed to simulate 1s of “a day in the life” of a polymer.

SUPERLION investigated a link between MD and a continuum mechanical model but the statistics in the MD did not contain enough ion jumps to be able to extract meaningful classical ion diffusion constants (D). The runs were exceptionally long - up to 6 months (shared time) on a "supercomputer" and the models contained up to 50 000 atoms - but nevertheless "MD box-sizes" and run-times were still too small/short to accumulate enough "ion-jump events".

Advanced methods have thus been developed to increase the sampling and to obtain a more accurate answer. The two main methods in this category are: kinetic Monte Carlo and temperature accelerated molecular dynamics.

Kinetic Monte Carlo (KMC) determines relevant states and transitions, computes transition rates, and simulates kinetics. KMC is a stochastic computational procedure that generates statistically correct state-to-state trajectories. It is based on the assumption that **all** transition pathways are known. The main steps to setup a KMC simulation are:

- Identify possible states and transition pathways
- Compute rates for these transitions
- Generate a correct state-to-state trajectory by randomly selecting pathways with a probability proportional to their rate
- Sample an escape time

Accelerated Molecular Dynamics (AMD) tricks MD into reducing the separation of timescales between fast and slow components of the dynamics and renormalizes the MD-time accordingly. In accelerated molecular dynamics (AMD), we try to maintain this
key characteristic, while using statistical mechanics to trick MD into making escapes happen sooner.

Accelerated simulation methods have been used to calculate diffusivities of charge carriers, band structure calculations for up to 10000 atoms (HIPERSOL) calculate adsorption including quantum effects of light-weight hydrogen (HYPOMAP).

Post-processing and Extraction of parameters

Models will produce values at many points in space and time and these results might have to be reduced into values representing a larger area. Post-processing is concerned with homogenisation for further use of the data in coarser models and in visualising the results or in the generation of constitutive equations.

DYNAMAG and MAGNONICS are using SEMARGL for post processing and data transfer, notably for covering the results of simulations performed in the time and real space domain to the frequency and reciprocal space domain.

FEMTOSPIN Is developing interfaces to transfer ab-initio information from various packages into atomistic codes and to transfer atomistic information into mesoscopic codes

METACHEM and NIM-NIL are calculating the EM field at many points in space and from these scattering, transmission and reflection parameters have to be extracted. Further processing is done into negative refractive indexes but the value of this notion is currently subject to debate.

SIMBA has developed software with which to describe nanopowder nucleation out of the gas phase. This is an aerosol model tracking the particle size-distribution and particle population in the reactor region and gives the precursor particle thermal history and trajectory prediction. The software then calculates the process yield.

Chapter 7
Model Development

7.1 Modelling of fundamental equations

The following projects added physics and/or chemistry to existing models. The definition of models and of model development can be found in the Introduction.

ARTIVASC

This project developed of a new equation to describe clogging and deposition of blood platelets.

ATHENA

This project developed first–principle models for complex oxides:
DFT extended with variational formulation of the pseudo-self-interaction correction scheme (pSIC)
new version of DFT exact exchange model
new hybrid Hartree-Fock DFT <describing what?>
method combining DFT with dynamical mean-field theory (DMFT)< describing what?>

AUTOSUPERCAP

Fast charge and discharge behaviour in a new model for the behaviour of battery-super-capacitor (or battery only) power systems.

CODICE

This project developed a new micro-level model for individual hydration of cement grains (HYMOSTRUC-3D). Also a novel Monte Carlo growth scheme to calculate aggregation of dried C-S-H particles was created, which provides a better insight than the existing phenomenological models.
The degradation model (CODICE_DEG) is a novel toolkit which solves the Nerst-Planck set of equations over a voxelized microstructal piece of cementitious material. By selecting sufficiently large voxels (but still within the nano-range) the code exploits the fact that the decoupling of the transport and chemical reaction equations is feasible. It enables to monitor the microstructural changes that take place along the degradation process.
A new fracture model enables virtual mechanical testing (e.g. tensile strength evaluations). It is based on a lattice beam formalism specifically adapted to the case of cement structures.

CRONOS

The project will make new descriptions of photo-energy conversion (combined electron-ion dynamics) and laser-induced ultrafast magnetisation dynamics. CRONOS will contribute to the development of TDDFT along four directions:
development of new DFT and TDDFT meta-GGA exchange and correlation functionals
development of new spin non-collinear DFT and TDDFT exchange and correlation functionals
development of method to combine non-adiabatic ionic dynamics with time-dependent DFT
development of optimal quantum control theory for TDDFT

DYNAMAG

Spintronic and thermodynamic aspects were added to an existing micro-magnetic model. Also the relative dynamics of different sub-lattices in ferri-magnets and antiferro-magnets and new spin-transfer torque mechanisms have been added to this existing model.

FEMTOSPIN

Optical spin manipulation and light induced magnetisation processes involving interactions between spin, conduction electrons and laser light have been developed in a new femto-scale model for exchange, spin-orbit coupling and spin-flip scattering, that can describe non-equilibrium spin-scattering (energy and spin transfer). The project developed a LLB equation for ferrimagnetic materials and parameterisation using atomistic models the new version has two sublattices to represent ferrimagnets and antiferromagnets. The two sublatttices give very different dynamics and allow exchange modes which we believe explain the thermally driven magnetisation reversal. Development of an entirely new 'heat bath' approach, in which the thermally excited heat bath (for example, the conduction electron population) is simulated and coupled directly to the spin system. A model based on the multiband Hubbard Hamiltonian to calculate exchange in disordered systems is also developed.

FIRERESIST

In FIRE-RESIST a 1-D finite difference model (COM-FIRE) based on the Henderson equation has been constructed to account for heat conduction (with temperature-dependent thermal properties), decomposition of the resin phase and the permeation of gaseous decomposition products through the solid structure towards the flame. Results from DSC (Differential Scanning Calorimetry) and thermo-gravimetry, provide the data for the decompositions and phase transitions that occur during heating of the resin systems. The model has been adapted and improved to describe: structural response of a particular composite component under load in fire, residual strength after fire.

GOFAST

The project will develop a model to describe the temporal evolution after being driven out of equilibrium by high-energy excitations (photo-injection by ultrafast laser pulses) in correlated materials (conduction in Mott insulators and superconductivity in cuprates.

HIPERSOL

HiperSol developed two completely novel schemes for the calculation of recombination rates. The first approach is based on Fermi's golden rule. Envelope functions are fitted to band structures obtained from first principles calculations of structures containing different kind of traps (e.g. strongly localised K-centres in the silicon nitride with Si atoms bounded to three N atoms instead of four). Also a model will be developed to obtain Auger recombination rates (the most important non-radiative process in semiconductors) from k-point interpolation of orbitals and eigen-energies using Gutzwiller techniques.

LEMSUPER

Many-body techniques for metal-insulator interfacesexist (e.g. Dynamical Mean Field Theory (DMFT) but generally assume spatial uniformity. The project will develop models able to describe inhomogeneous situations and will apply these to surface doping.
This may be done by assuming that the electron self-energy depends, besides on the frequency, also on the layer depth below the surface plane. Dividing the space below the surface into layers the self-energy will be calculated by solving an auxiliary impurity model for each layer in which the conducting bath depends self-consistently on the fully interacting impurity Green's functions not only of that given layer, but also of the nearby ones. The effect of many body interactions beyond mean-field levels in picene and similar molecular

systems will be added to the models. Improvements to the modeling of new superconducting materials will include Gutzwiller correlations, applying a method recently developed (before Dynamical Mean Field Theory).

MONAMI

The project developed a theoretical technique for calculating the effect of electron-electron correlations. The developed models are an elaboration of existing models to make the theory general to treat complex crystal structures like that of V2O3.
Non–Newtonian dynamics (temporal evolution of a system of classical objects) are incorporated in UppASD package for spin-dynamics in order to describe the behaviour of nano-sized magnetic systems of particular symmetries.

Also an extension was made to allows accurate and fast calculations of ground state properties of solids by incorporating tail cancellation of orbitals. This is base on physical insight in how electrons move around in solids, and how to best describe their quantum mechanical equation of motion. In the model developed in MONAMI, several conceptual steps and mathematical derivations have been made to come to a set of equations which enable a numerical implementation.

MORDRED

Models have been developed for statistical impact of bias temperature instabilities and hot carriers on the electrical characteristics of CMOS transistors. Also a model for the impact of local defect generation on dielectric gate leakage current is developed.

NAMASTE

The project has implemented relativistic corrections (i.e. spin orbit coupling) to the band structure calculations of diluted ferromagnetic semi-conductors (DMS). (no codes to do so existed yet). They have subsequently used these tools to: a) describe the magnetic anisotropy of DMS, b) explore how magnetization and anisotropy change either varying the total electron carrier density or strain acting on the films/nanostructures; c) predict a new batch of antiferromagnetic metals with strong spin orbit coupling (antiferromagnetic materials for spintronics) and d) to describe single electron transistors.

NIM_NIL

A EM model was developed to describe the dissipative loss in resonant electromagnetic metamaterials. The model takes into account the radiation damping of the resonant currents, which is necessary to model metamaterials made from low-loss conducting materials. This model led to an identification of which conducting materials are useful for metamaterials. Silver was found to be the best conducting material at optical wavelength. Graphene was ruled out.

OXIDES

This project has developed models using pSIC and B1-PW wave functions.

RADINTERFACES

Irreversible processes leading to material damage taking place under irradiation described by a new hybrid kinetic Monte Carlo-Molecular Dynamics model. This Object Oriented kinetic Monte Carlo (OKMC) method allows to follow the evolution of individual defects (i.e. vacancies, interstitials, He and their clusters) by listing all possible reactions and paths that a given defect could follow and choose the most probable one based on a statistical method (allowing the use of longer time step). All possible events are quantified using migration

energies, formation energies (leading to binding energies). These energies are quantified using Nudged Elastic Band method in Molecular Dynamics.
A damage accumulation model is also developed based on differential equations to describe the thermodynamic and kinetic response of the synthesized materials to microstructural features. This is a 3 Dimensional Cluster dynamics model -where transport and reactions in the form of absorption and emission of defects are taken into account. In this model, rather than following individual defects within the nanloayered system, defect quantities are followed as densities. This leads to a great decrease in the amount of information (i.e. defects) to be followed which then allows to simulate the evolution of defect for long time scales.

SIMBA

An existing model for plasma fluid-dynamics for nanoparticles production has been extended to simulate non-equilibrium plasma allowing low pressure operating conditions and strong temperature gradients due to the quenching system.

ULTRAMAGNETRON

Basic physics for opto-magnetic reversal process have been added to an atomistic Heisenberg model. These describe the thermal processes involved.
The single-macro spin Landau-Lifshitz-Bloch model was extended into a multi-macro spin model taking the exchange coupling as well as the dipolar interaction into account.

7.2 Modelling of constitutive equations

MATRANS developed a new constitutive model defining the relationship between tensile strength of functionally graded materials (FGMs) and volume fraction of ceramic phase has been developed to simplify complicated mechanical behaviour of FGMs.
In oxidation modelling a new constitutive relation has been proposed between the oxide growth rate and the surface temperature. Since the calculated macro temperatures are too low to allow for the oxidation, only closer look at surface asperities can provide the mathematical model for the experimentally observed oxidation phenomena. A user-defined FORTRAN code for the developed constitutive relation has been added to a commercial FE software.

MODIFY developed new macroscopic constitutive equations capable of describing quite reliably the deformation equations (e.g., the shear and elongational behaviour) of the synthesized PSA materials. The new equation utilizes generalized expressions for the strain energy density as a function of the three invariants of the conformation or deformation gradient tensor. In limiting cases, it reduces to known laws widely used to describe hyper-elastic materials, such as the Rivlin-Saunders and Hart-Smith theories.

MULTIHY has developed macroscopic models based on novel set of constitutive equations for H diffusion capable of exploiting the information being derived from the atomistic calculations. The equations are more generalised than those commonly used in the literature, enabling the description of hydrogen diffusion under a broader range of conditions (e.g. temperature variations, trap occupancies) as before.

POCO developed an electro-dynamics constitutive equation relating the polarisability of the CNTs, the electric field applied and the viscosity of the polymer with the torque.

ROLICER extended existing models that treat damage and fracture in silicon nitride to include under cyclic contact loading based on the behaviour of the solid phases and boundaries phases.

Chapter 8
Modelling applications

This chapter will be expanded soon.

Project	Topic of models	APPLICATION (sector)	APPLICATION (product)
ADGLASS	Protein adhesion, interface cohesion and crack propagation in glasses	Energy	Glass products for pharmaceutical and photovoltaic applications
AMCOS	Zeolitic imidazolate frameworks, hyperbranched aminosilicas, functionalised polymers: advanced materials for selective sorption of carbon dioxide from gaseous mixtures.	Chemistry	Capture of CO2
AMON-RA	carrier transport and bandgap in III-V Semiconductor material	Energy	Solar cells and optoelectronics
ARTIVASC 3D	blood and nutrient transport in vascularised biomaterials	Health	Regenerative medicine
ATHENA	Transition metal oxides (magnetic perovskites, double perovskites, diluted magnetic ferroelectrics, piezoelectrics, magneto resistivity heterojunctions, superlattices and multilayers)	ICT	IT devices

AUTOSUPERCAP	Battery-supercapacitor power system for an electric vehicle (EV) application Ion transport in supercapacitors made of carbonaceous materials, e.g. activated carbon, carbon nanotubes, graphene	Automotive	Automotive
CODICE	cement hydration	Construction	Construction
CRONOS	Energy photo-conversion and laser-induced ultrafast magnetization dynamics	Energy/ICT	Solar cell, IT devices
DISC_REGENERATION	Biomaterials and vascular transport in intervertebral discs	Health	Biomedical implants
DYNAMAG	spin dynamics in magnetic material (scattering, absorption and emission)	ICT	IT devices
FEMTOSPIN	Heat-assisted or optically induced ultrafast reversal of magnetism	ICT	IT devices
FIRE RESIST	fire resistant polymer matrix composite materials	Construction	Manufacturing industry
FREECATS	Catalysis reactions and processes in foam structures	Chemistry	Metal-free catalysts
GOFAST	Optical control by intense ultra-fast laser pulses of metallic phases in the prototypical Mott insulator V2O3 and of the superconductive phase in the high-temperature superconductor family BSCCO.	ICT	IT devices
HIPERSOL	Resistance and recombination of charges at interfaces in solar cells	Energy	Solar cells

HIVOCOMP	Composites consisting of a matrix and textile fibrous reinforcement (woven carbon fabric) and self-reinforced composites	Transport	Transport, aviation
HYMEC	organic semiconductor	ICT	Photonics and electronics
HYPOMAP	Hydrogen storage materials (physisorption and chemisorption), ad- and desorption processes, and proton exchange membranes.	Energy	Hydrogen storage
IMS&CPS	Textile carbon fibre/epoxy composites reinforced with carbon nanotubes (CNTs), damage resistance, electrical conductivity and lightning strike protection	Transport	Transport, aviation
INNOVASOL	Excitonic solar cell materials (QuantumDots, Transparant Conductive Oxides and solid electrolyte)	Energy	Solar cells
IRON-SEA	tunneling and reflection in Fe based superconductors	Energy	Superconductors (Josephson devices and SQUIDs.)
LEMSUPER	Light element superconductivity	Energy	Superconductors
MAGNONICS	Spin dynamics of magnonic metamaterials	ICT	Spintronic devices
MASTER	Spin wave excitation by spin-polarized current and spin-diffusion effect in normal metal near a junction	ICT	IT device
MATRANS	Properties and behaviour of metal-ceramic functionally graded materials	Transport	Transport, aviation, automobile

METACHEM	Electro-magnetic characterisation of nano-structured metamaterials	ICT	IT devices
MINOTOR	electronic phenomena at interfaces in organic-based electronic devices	ICT	OLEDs, transistors, sensors and storage devices, solar cells
MINTWELD	welding processes of metal alloys	Manufacturing	Welding failure prevention
MODIFY	stress-induced deformation of adhesive materials	Manufacturing	Adhesives
MONAMI	Molecular- and nano-magnetism, spintronics and magnonics, Quantum transport through materials at nano-scale, magnetism	ICT	ICT devices
MORDRED	oxide interfaces with ferrolectric or multiferroic properties	ICT	IT devices
MULTIHY	Microstructure and mechanical properties of materials under the effect of hydrogen embrittlement	Manufacturing	Degradation prevention
MUST	Inhibitor release, self-healing mechanisms and nanocontainers, formation of containers with membrane emulsification, multifunctional coatings	Transport	Self-healing coatings
NAMASTE	manipulation of magnetic materials by electric fields and strain	ICT	ICT devices
NANOINTERFACE	adhesion of and interface fracture in metal-oxide-polymers	ICT	Electronic devices
NANOMAGMA	Magneto-optic metallic nanostructures	ICT	IT devices

NANOMODEL	Mechanical, thermochemical and flow behaviour of nano-filled polymeric materials	Chemistry	Reinforcement of polymers
NEXT-GEN-CAT	catalysts of metal nano-particles with transition elements but without Platinum Group Metals (PGM)	Transport	Catalysis for engines
NIM_NIL	electromagnetic characterisation of and loss reduction in metamaterials	ICT	Optical devices
NPMIMETIC	biomimetic nano-polymer for disc regneration treatment	Health	Biomedical implants
ONE-P	Electronic processes occurring in organic-based devices	ICT	OLEDs, transistors, sensors and storage devices, solar cells
ORAMA	Multifunctional oxides (Active Semiconductor Oxides (ASO)) Passive n-type amorphous Transparent Conducting Oxides (a-TCOs) and p-n type junctions thereof	ICT	Electronic devices for automotive
OXIDES	Oxide interfaces and nanostructures (structural, electronic and functional properties)	ICT/Energy	ICT devices, energy harvesters
POCO	mechanical behaviour of functionalised carbon nanotubes in polymer matrices	Transport	Structural parts for automotive, aeronautics, building, aerospace, wind power generation (blades), ship building, biomedicine

RADINTERFACES	Damage mechanisms and effects on mechanical properties for novel crystalline materials with large interfacial areas	Construction	Prevention of nuclear radition damage
REFREEPERMAG	magneto-crystalline and shape anisotropy of RE-free magnets	ICT	Magnets
ROLICER	Damage and degradation of ceramics (silicon nitride, mechanical and thermal loading)	Manufacturing	Coatings for bearings
SIMBA	plasma transport and thermodynamics in an inductively coupled plasma synthesis technique	Chemistry	Production technique for battery anodes
SIMUGLASS	fluid dynamics in precision glass moulding	Energy	Glass moulding for optical devices
SMASH	strain, polarisation and quantum effects in GaN nanocolumn LEDs	Energy	LED
SSEEC	Magnetic materials, micromagnetism, magnetic cooling engines	Energy	Refrigeration, airconditioners
SUPER-IRON	physical properties of Fe based superconductors	Energy	Superconductors
SUPERLION:	Nano-architectured battery materials and 3D microbattery components	Energy	Microbatteries for electonic devices
SURFUNCELL	adsorption phenomena at cellulose surfaces	Chemistry	Paper, membranes, textile, films
ULTRAMAGNETRON	optical control of nanomagnets	ICT	IT devices

Chapter 9

Impressions of Industrial modelling

The NMP Programme has as objective to support industrial technologies. This chapter presents how companies involved in NMP Materials projects are using models.

> *Please note that these are impressions and not necessarily a complete account of what these companies do.*

Industrial areas

The responding industries are operational in the following industry sectors:

- chemical, materials research (BASF)
- transport (BMW)
- energy efficient, gas-free refrigeration and cooling technology (CAMFRIDGE)
- near net shape composite technologies for aeronautics (COEXPAIR)
- polymer manufacturing (DOW)
- aeronautic and space industry (EADS)
- magnetic and optical systems, crystal growth (INNOVENT, Department of Magnetic and Optical Systems)
- chemicals and polymer manufacturing (LYONDELL-BASELL)
- chemistry (MERCK)
- automotive transmission systems (OERLIKON DRIVE SYSTEMS)
- manufacturing of ICT devices (OXFORD INSTRUMENTS)
- manufacturing of ICT devices (PHILIPS)
- risk technologies (RISK-TECHNOLOGIES)
- cutting tools for grinding, milling and drilling (SANDVIK COROMANT)
- chemicals, processes, materials research (SOLVAY/RHODIA)
- solar energy (SOLARONIX)
- steel manufacturing (TATA STEEL)
- energy, security (explosion), manufacturing (TOTAL)
- materials technology / chemistry / material sciences (UMICORE)

Type of models used

The models used span all classes of modelling (electronic to continuum modelling)

The reason why industry uses modelling

BASF uses modelling as it offers unique insight and modelling is considered to allow for faster development cycles (guide to experiments, interpretation of experiments).

BMW wants to reduce development time, development cost and hardware for testing.

CAMFRIDGE states that modelling helps them design their products more quickly.

COEXPAIR is using modelling to design composite parts for aeronautics applications by analytical and numerical calculations and models. They so ensure that the composite part can withstand the loads occurring during flight of the aircraft.

DOW uses modelling as it speeds up development of new products and provides insights into application properties of materials.

EADS wants to gain process knowledge, shorten lead time, replace time and cost expensive trials.

INNOVENT uses modelling as it is often the only available mean to understand intrinsic properties and behaviour of magnetic, optical and semiconducting materials and it saves time and money when designing new device prototypes.

LYONDELL-BASELL predicts final product properties and performance with modelling. They also limit experimental cost and minimize time to develop new products, understand and control industrial processes.

MERCK predicts specific material properties as a form of pre-screening.

OERLIKON predicts the effect of the transmission system design on vehicle performance and energy efficiency with modelling.

PHILIPS uses models to understand the underlying physics of devices and processes; to optimize product designs and processes, to shorten development and qualification time and to decrease the time-to-market.

RISK-TECHNOLOGIES uses multi-scale modelling of corrosion protection for new materials, testing and optimisation of new materials and new devices.

SANDVIK COROMANT uses models to gain deeper understanding of the materials properties of i.e. hard cutting tools and to enable faster development of new products. FEM modelling of the cutting tool process is used to save time in machining tests and to better understand the wear behaviour of the cutting tool. One common method is the prediction of phase diagrams (ThermoCalc), but also, the energetics and geometry of metastable compounds or compounds where no/little experimental

data exists can be calculated by first principles software such as VASP, Phonopy etc. CFD and other methods are used to simulate synthesis processes in order to save time and improve understanding of these processes.

SOLARONIX states that modelling helps to optimize solar equipment. Modelling helps screening new materials by discarding the ones that are not compatible seen their energetic levels.

SOLVAY/RHODIA uses modelling to catalyse and support all stages of its innovation processes and to continuously improve the operational performance of its production technologies. Modelling is a key part in SOLVAY/RHODIA to understand, predict, design, optimize and control, which highly complements experiments.

TATASTEEL have been using modelling through the years in various R&D activities, such as materials design, processing route selection and optimisation. Recently, they have benefited from their weld modelling and simulation exercises in terms of understanding and control of weld induced residual stresses and distortion, as well as avoidance of formation of unfavourable microstructures in critical areas such as heat affected zone. They also use modelling to complement our physical experiments and generate inputs for engineering critical assessment work of structures in service.

TOTAL uses modelling to understand the behaviour of certain materials under well-controlled conditions and to study physic-chemical properties of compounds, thermodynamics, CO2 storage, new active compounds (polymers and lubricants, etc.) for interface activities.

UMICORE uses modelling as it can speed up considerably the design time for new processes (faster screening of alternative designs). It helps to optimize the efficiency and performance of processes by giving a more thorough insight in the physics involved, which will facilitate the debottlenecking. The use of modelling can also help to reduce the number of required experimental tests, thereby reducing the overall costs.

Industrial use of models for new materials

BASF uses these models for rapid screening and simulated tests of quantum chemistry (reaction mechanisms, kinetics, photo-physics, new chemistries), complex liquid mixtures (formulations) and organic semiconductor properties (e.g. exciton or charge carrier mobilities).They are working on homogeneous and heterogeneous catalysis (mainly quantum chemistry) quite extensively! Also theoretical thermochemistry is an important topic (including high level methods like CCSD(T)). We are also using Hybrid-QM/MM-approaches for catalysis (mainly enzymatic reactions) from time to time and there is now some revival of these methods with respect to organic semiconductors. Besides that theoretical photochemistry/photo-physics is an important topic.

DOW uses materials modelling going from molecular structure to processing and end-use properties, and back. They do fundamental modelling of reaction mechanisms, rheology, interfacial behaviour and self-assembly; rational design of formulations.

EADS: newly developed alloys lack a proper description in terms of constitutive laws necessary for FE simulation studies. EADS uses new and self developed models to validate such new materials and get more insight into its behaviour during manufacturing operations.

INNOVENT does simulations of static and dynamic behaviour of patterned magnetic films and magnetic nano-composites in order to understand the results of corresponding measurements and predict the properties of new magnetic materials. They also use (home-made) software for simulating dislocation dynamics in crystals.

LYONDELL-BASELL calculates material parameters from rheological and other physical tests, predict rheological properties from chemical structure, compare theoretical predictions to experimental results.

MERCK uses materials models for the estimations of electronic energy levels (e.g. HOMO / LUMO) in molecules / polymers.

RISK-TECH uses dedicated Molecular Dynamics, Dissipative Particle Dynamics, Computational Fluid Dynamics, continuum mechanics, fluid-structure interaction software for simulated test of new materials and as the software allows optimising of the fitting parameters they can determine the optimal material characteristics. They e.g. analyse the effect of varying the nanocontainers fillings, particle-particle interactions, diffusivity parameter and the localization of the particles into the scratch. These findings provide guidelines for formulating nanocomposite coatings that effectively heal the surfaces through the self-assembly of the particles into the defects.

SANDVIK COROMANT uses electronic structure methods like VASP/VASP+phonopy to calculate thermodynamic properties, geometry and electronic structure of compounds used in the bulk and coating of the cutting tools. Empirical models based on large sets of measured data are used to predict mechanical properties of the cutting tool.

SOLARONIX calculates the energy levels in new solar cell material.

SOLVAY/RHODIA is oriented toward a computer-aided rational design and optimisation of new highly functional materials and formulations for sustainable solutions in the fields of energy, consumer chemicals, electronics, automotive, ... Molecular modelling (ranging from electronic to meso-scopic scale) and empirical modelling are used to perform a virtual and high throughput experiment screening of new materials as well as to pinpoint the most important microscopic material properties which (qualitatively or quantitatively) determine the macroscopic performance and application properties. Also, they are a valuable tool to establish new design concepts that can enlarge the discovery process and help experimentalists in their daily work. End application behaviours are simulated (e.g. with Finite Elements) in order to optimise the solutions that are delivered. Process technologies used to produce these materials are also simulated (e.g. reaction kinetics, computational fluid dynamics, heat integration, dynamic process modelling) to design eco-efficient processes which minimize the environmental footprint and reduce associated CAPEX and OPEX.

TATASTEEL uses materials modelling for thermodynamic and phase diagram calculations (during solidification and heat treatment) and microstructure prediction during thermo-mechanical processing of steels.

TOTAL study materials properties and absorption capacity, enhanced oil recovery, polymers development, additives for lubricants or fuels, friction studies and corrosion.

UMICORE simulate the mechanical strength/service life of new materials in specific customer applications.

Industrial use of models for manufacturing

COEXPAIR is using visualisation models to generate and visualise the finite element model before and after calculation. They use analytical modelling and continuum mechanics models to calculate stress, deformations, displacements of composite parts such as T shape junctions or I shape beams up to the complete final part e.g. the landing gear door of an aircraft.
With these they do analysis of deformation and stress in the material loaded with a static or dynamic mechanic load, thermal load, thermo-mechanic load, vibration load for resonance and instability.

EADS uses Finite Element based software for process development to optimize part accuracy or process parameters during metal forming or machining.

INNOVENT uses (home-made) software for simulating crystal growth and dynamics of point defects in crystals.

LYONDELL-BASELL: uses modelling for reactor engineering and process engineering, checking proper functioning of the reactor and predicting final product structure and material performance at customer-applications.

OXFORD-INSTRUMENTS models processes in order to optimise their design of new plasma etch and deposition hardware.

RISK-TECHNOLOGIES use two different modelling approaches for self-healing materials consisting of nano-containers. Simulation determines nano-containers fillings, particle-particle interactions, diffusivity parameter and the localization of the particles into the scratch.
The models are Dissipative Particle Dynamics, Finite Element Method and continuum mechanics.

SANDVIK COROMANT uses CFD-modelling as well as other internally developed methods to simulate manufacturing processes.

SOLVAY/RHODIA uses modelling for the sustainable improvement of the operational performance of its manufacturing units, looking for optimizing capital and operational expenditures. Computational fluid dynamics is used to troubleshoot, debottleneck, re-vamp process equipment and to optimize their overall efficiency. Heat integration is performed to make efficient use of energy. Advanced

process control solutions are used to operate processes as close as possible to the optimum limits while satisfying safety constraints and ensuring that quality requirements are met. Statistical data mining is used to value plant historical production data coming from manufacturing execution systems so as to identify and optimize key process variables. Dynamic process modelling allows building Operator Training Systems to develop skills of manufacturing teams. Polymer processing technologies that are used by our customers are also simulated to bring them our knowledge of our materials.

TATA STEEL uses manufacturing models for loading and deformation prediction in rolling and pipe forming, characterisation of residual stress and distortion due to welding, prediction of microstructure and properties in thermo-mechanical processing of steels and assessment of in-service performance of steel products and Computational Fluid Dynamics.

TOTAL uses models for polymers compounds manufacturing processes.

UMICORE is simulating metallurgical and chemical processes ranging from a single operation to entire plants. It is used to debottleneck and troubleshoot manufacturing processes. The models are often used to reduce the number of measurements and to design efficient experiments. They also do verification of new designs of processes (i.e. ovens, gas treatment plants,…).

Industrial use of models for products/devices design

BMW uses computational fluid dynamics and crash, fatigue and stamping simulation to predict the behaviour of their cars.

CAMFRIDGE use software to optimise device architectures by optimising geometries for heat transfer, fluid flow, magnetic force maximisation, magnet design. The code is integrated with CAD design tools – "really it is our SWISS army knife".

COEXPAIR is using the same approach for product design as they do for material design (visualisation models and continuum mechanics models to analyse deformation and stress in a composite part loaded with a static or dynamic mechanic load, thermal load, thermo-mechanic load, vibration load for resonance of the part and instability).

INNOVENT uses models based on electromagnetic field theory and mesoscopic theory of ferromagnetic materials to optimise permanent magnets and current circuit configuration in order to achieve the desired magnetic field configuration.

OERLIKON uses Finite Element Analysis, CFD, general computing software and multi-physics modelling software for the design of the mechanical parts, the optimisation of the transmission internals (churning losses) and the evaluation of the impact of the transmission system design on the overall vehicle performance.

SANDVIK COROMANT uses FEM modelling to simulate the cutting tool process and predict wear behaviour at different process conditions. The utilization of first principles modelling to simulate the chemical interaction between the cutting tool a work-piece material is at an early stage pf development.

SOLARONIX uses solar illumination simulation software and device design software for the design of microwave wave guides and antenna's.

SOLVAY.RHODIA uses modelling tools to predict and validate relationship between parameters to prepare and synthesize product versus final properties.

PHILIPS applies new and existing models to predict the physical behaviour of current and future devices thereby taking into account the processing history. After experimental validation, the models are applied to achieve optimized product and process design with respect to several failure mechanisms such as interface cracking and fatigue. The models deal with thermo-mechanics, fracture mechanics, multi-scale mechanics, heat transfer and multi-physics phenomena.

TATA STEEL carries out system design, optimisation and performance evaluation of a novel (mechanical) device (machine) for weld (hot) cracking susceptibility testing with the models.
RISK-TECHNOLOGIES develop the computational procedures and software for modelling of blood flow in micro-vessels and particle margination and endocytosis. A general scheme of the physical process involving blood microcirculation, nanoparticle motion, attachment and endocytosis is modelled using continuum-based methods

TOTAL uses chemical engineering models for simulation of reactors and processes and apply this a.o. to multiphase-multi-fluid flows, flows in porous media and combustion.

UMICORE does design optimisation of new devices with respect to efficiency and /or mechanical strength/service life.

Industrial research into modelling

BASF is doing development of multiscale modelling, both vertical (parameter estimation from chemistry to coarse graining) and horizontal (coupling of continuum mechanical modeling and particle based MD). Related to organic semiconductor research quantum chemical parameters for intermolecular interactions relevant to charge and exciton transport as well as drift diffusion models are focus of research. They participated in an EU-project QUASI, where they were co-developing the software Chemshell.

DOW does research into a large variety of simulation routines in polymer science.

LYONDELL-BASELL is developing reaction engineering and polymerization kinetics for their own processes in order to achieve process optimization

INNOVENT participates in research into numerical methods in micro-magnetics, in order to increase the efficiency of existing packages and to develop new packages for simulations of those classes of magnetic material which can not be simulated with the state-of-the-art software. They also do development of the software for simulations of the dislocation dynamics in crystals in order to understand the formation of equilibrium and non-equilibrium dislocation patterns in semi-conductors.

OERLIKON is doing simulations based on newly developed vehicle models and energy managements system models, actuation system models, churning and windage losses models.

OXFORD INSTRUMENTS is developing new atomic and molecular chemical reactions sets to be added to their plasma modelling code.

PHILIPS is doing research into fracture and damage mechanics, multi-scale mechanics and thin film mechanics.

RISK-TECHNOLOGIES develops computational procedures and software for modelling of blood flow in micro-vessels and particle margination and endocytosis. They developed two different modeling approaches, DPD and FEM for self-healing materials, based on the nanocontainers healing concept.

SANDVIK COROMANT develops empirical/semi-empirical models of mechanical properties of hard materials and performs thermo-dynamical assessments of new materials ´systems. Models for manufacturing processes are continuously developed and improved.

SOLVAY/RHODIA has internal R&D activities and external partnerships in the modelling of catalytic reactions, reactive and multiphasic flows, multi-physics and multi-scale simulation of advanced materials, development of quantitative laws for predicting materials and blends properties.

TATA STEEL is developing industrial scale modelling of welding for weld induced residual stress and distortion characterisation, incorporating the capabilities of defect prediction such as cracking using multi-scale modelling techniques.

TOTAL develops models for multiphase flows in risers (avoid Hydrates), and derives closure equations of "slug flows".

Chapter 10
Achievements of the models

Of course the results of all the models are very impressive and useful for industry.
In this chapter a subset of these results is presented, listing those achievements that can NOT be achieved experimentally. It is hoped that this can convince experimentalists of the value of modelling!

ADGLASS

The modelling revealed previously unknown details of an important process (hydrogen embrittlement of silicon crystals) widely employed for the fabrication of Silicon-On-Insulators (SOI) nanoelectronic devices. It also unveiled undiscovered mechanisms of brittle fracture in solid materials, including the precise chemomechanical role of defects (impurities, reconstructions, dislocations) and dynamical instabilities during the propagation of cracks in brittle materials. Moreover, the simulations explained the reasons for the previously observed, yet so far very poorly understood, binding specificity of certain peptide sequences to inorganic materials surfaces. They revealed an unknown adhesion driving force modulated by the local variations of water density at the solid/liquid interface.

AMCOS

Simulations can predict the sorption isotherms of pure and mixed gases in recently synthesized nanoporous materials (zeolites, metal-organic frameworks, polymers), or in hypothetical materials considered for synthesis. They can also predict the rates of diffusive transport through these materials.

AMON-RA

The model guides device development by

- Definition of suitable bandgap energies for single- and dual-junction nanowire solar cells
- Definition of suitable device structure including doping levels and barrier layers
- Definition of optimum configuration for wire length, distance and diameter in nanowire array
- Understanding of optical and electrical loss mechanism in single- and dual-junction nanowire solar cells

Contribution to roadmap for assessment of III-V nanowire photovoltaics

ARTIVASC-3D

The hydrodynamic modelling will be able to predict wall shear stresses at the vascular graft walls. These stresses have to be within a certain range in order to stimulate the endothelial cells to perform e.g. neo-angiogenesis.. These wall shear stresses would be

extremely difficult to measure for any possible graft geometry. Therefore, a modelling-based design approach is crucial for tissue engineering.

ATHENA

Identification of candidate materials and materials interfaces for future nano-electronics based on complex oxides. These included hetero-junctions, superlattices and multilayers consisting of doped magnetic perovskites (e.g. LaxSr1-xMnO3, PrxCa1-xMnO3), double perovskites (e.g. LaNi1-xMnxO3) and diluted magnetic ferroelectrics designed to exploit and manipulate the coupling of different order parameters at the two sides of the interface.

Prediction of the phase diagram of complex magnetic oxides MnO and NiO under pressure,

Explanation of the extremely high antiferromagnetic ordering temperature in SrTcO3 and BaTcO3.

AUTOSUPERCAP

The battery-supercapacitor modelling and simulations allow selection of the best materials/supercapacitor for scaling up reducing experimental costs.

The molecular ion simulations guided the research for a pore size, maximising the specific capacitance for carbonaceous electrode materials and thereby increasing energy and power density.

CODICE

The developed toolkits revealed that there is a synergy in the hydration of alite and belite phases of cement clinker, which opens the door to new eco-cements.

While a priori one would expect that the larger the content of C_3S the better the resulting mechanical properties, the simulations have revealed that there is synergy in the hydration of C_3S and C_2S blends, and that there is an optimum C_3S/C_2S ratio around 70/30.

DISC-GENERATION

The modelling contributions are twofold:

The coupled transport-mechano model is able to predict the movement of solutes within the intervertebral disc and predicts the interactions between mechanical properties, fluid and solute transport, and cell viability. This is essential for a proper understanding of the mechanisms of disc degeneration and disc regeneration with the use of biomaterials as disc substitute.

Simulations of the effect of partial and complete disc nuleotomy on load transfer as a function of the biomaterial substitute used can be used to determine the surgical variability during nucleus removal.

Both contributions cannot be obtained experimentally and therefore are complementary to the experimental evaluation of the biomaterial performance.

DYNAMAG

The calculations pointed out samples that were until then simply not considered.
A novel magnonic logic architecture has been developed based on physics discovered by the models.
The, until then unexplained, origin of the response experimentally observed in optical pump-probe studies of magnetic multilayers with strong perpendicular magnetic anisotropy, has been revealed via calculations in the discrete lattice model.
Mechanisms behind unusually low magnetic domain wall depinning currents within spintronic devices have been revealed via full 3D finite element simulations.

FEMTOSPIN

Prediction efficiency of ultrafast spin dynamics in multiferroics excited by THz laser pulses
Prediction of the smallest stable domain structure in magnetic thin films
Prediction of the time and spatial scales of magnetic pattern formation
Identification of optimal materials for ultrafast optically induced magnetic switching

FIRERESIST

Modelling can predict in the solid phase, the temperature and degree of resin decomposition at any point within the structure, data not accessible for measurements. This is then used in the design of fire-sensitive structures for use in transport applications with a minimum amount of costly testing.

FREECATS

Heat transfer modelling guides the design of the foam materials and predicts the deposition of carbons during operation, (a phenomenon critical in oxidative dehydrogenation) and so reduce costs of trial and error developments.
Multi-scale modelling of reaction, surface-fluid interactions, heat transfer and hydrodynamics allow to predict from first principles the behaviour of the overall reactor system and to screen a large space of operating conditions prior to experimentation. This leads to better understanding of physical phenomena involved and dynamics of processes within the system, thus reducing the number of experimental trials required.

GOFAST

The model identified optimal correlated materials (composition, size, direction of the laser pulse versus surfaces, etc...) and excitation pathways (photon energy, intensity, polarization and temporal profile) for the production of controllable and reversible photo-induced transition between very distinct phases, e.g. metallic and insulating, or normal and superconducting.

HIPERSOL

The methods can predict contacting and recombination properties of nanostructured materials and complicated interfaces.

The model gave fundamental insight into nitrogen diffusion in silicon, into the nature of different recombination traps, into dissolution and transport of Ag during the firing process, and insight in how the current flows through the contacting region. Based on this optimal Ag crystallites geometries were gained.

HIVOCOMP

Prediction of structural properties to avoid unfeasible or expensive experimental tests. The models also enabled screening of possible choices for the resins. The flow modeling shortened part of the design by predicting permeability and impregnation time of the different resins.

The model predicted structural behavior in function of the above properties and damage initiation by calculating the threshold and damage development parameters in the composite during different loading types

HYMEC

The electric field distribution of charged metal nanoparticles in organic matrices can be predicted, which allows identifying the switching mechanisms of memory cells. This, in turn, allows optimizing the morphology of devices.

HYPOMAP

Computational modelling, in particular on the electron or atomistic scale, allows the investigation of processes beyond the experimental scale. People often speak of the "computer microscope" that allows to monitor the motion of a single atom. It also provides understanding of an individual vibrational mode, or of the contributions of material fragments to an individual property. In this project modeling provide insight in the adsorption energy of hydrogen as function of the composition of the individual building blocks of a molecular framework. With this data it is possible to improve the performance of the target materials.

IMS-CPS

The "electrical conductivity" model predicts the electrical percolation and conductivity of CNT/polymer composites close to the experimental observations. The achievements beyond experiments include the positive effect of agglomeration and the transverse conductivity of the CNT/polymer composite with the CNTs only sprayed on the surface. In fact, nobody believed that there will be conductivity in the transverse direction when the CNTs are sprayed on the surface alone. In addition, this model correctly predicted that the addition of compatibilizers and copolymers has a significant effect on electrical percolation threshold and conductivity. These characteristics are experimentally proved and this is the only model which can predict this behaviour.

The toughness model will predict the effect of carbon nanotubes and their agglomerates on re-distribution of stresses and strains inside the composite and the threshold strain for the onset of damage on the micro-scale.

The model utilized for validation elements can predict the initial failure of the T junctions and of the I beams for the different used materials (with and without CNT). This will help to design the test jigs to be used in the project.

INNOVASOL

Trial and error synthesis costs were avoided by computing the energetics of inclusion of some anions (iodide and tri-iodide) in a layered solid analogous to hydrotalcite before the actual systems were synthesized. The calculations showed the limit concentration expected for anions in this environment.

The models could provide understanding of phenomena occurring, e.g. the excess of lead observed in certain conditions.

The calculations allowed to predict which surface passivant would help obtain particles of octahedral shape exposing (111) crystallographic faces, and this will guide the experiments.

IRON-SEA

The model determined the pairing symmetry and its evolution with doping, which is impossible to determine experimentally.

The model determined the characteristic energy of the boson that mediates superconductivity (examples: Co-doped Ba-122, Sm-1111) and of the coupling strength.

The model determined the effects of disorder, doping, lattice strain, etc on the superconducting properties.

The model determined the effects that are optimal or detrimental for device fabrication and optimization.

LEMSUPER

New correlation-driven mechanisms for superconductivity in light element systems were predicted long before they were validated. A superconductivity mechanism for fullerides was predicted, where electron-vibron coupling, orbital degeneracy, and strong electron correlations implying a nearby Mott transition all play a crucial role. Cesium fullerides validated this theory.

Identification of new electronic ground states in light element systems leading to superconductivity, potentially unveiling new light element molecule-based superconductors, something that cannot be done experimentally.

MAGNONICS

Numerical simulation of quasistatic magnetization processes explain measurements by MOKE and of spin-wave excitations observed by FMR, BLS, and TRSKM techniques in 2D arrays of nanoscale magnetic dots and antidots. These simulations facilitate explaining the nature and spatial structure of magnons in the magnonic arrays.

MASTER

The model can predict the magnetization dynamics in an array of hetero-structures. These dynamics cannot be computed analytically. These simulations are used to optimize the design of spin devices as optimization by experimental means would be too costly.

MATRANS

Most of the modelling in the project is done to replace the experiments, which are usually complex and costly or, in other words, the modelling predicts the materials' properties/behaviour which will be observed in experiments and thus shortens the development process.

METACHEM

The model predicts whether the metamaterial can be described within effective media theory.

The model extracts parameters not directly measurable.

The model can determine individual polarizabilities of a complex scatterer (electric and magnetic), surface susceptibilities of metasurfaces (electric, magnetic and magnetoelectric), efractive index of the wave in a lattice and wave impedance of the wave in a lattice.

MINOTOR

Modelling allows material design of multilayer devices with optimized proprieties as follows:

- The model has predicted the contributions to the discontinuity between the electronic structure at the interface and the bulk material
- The model explained the origin of the electronic level alignments at organic/organic interfaces as measured in short-circuit current and the open circuit voltage of solar cell devices, two key quantities that directly dictate the efficiency of those cells.
- The model has shown that modifying the surface of electrodes, can tune the charge or spin injection barriers in devices such as OLEDs.
- The model predicted the influence of lattice mismatches at the interface between two crystalline organic semi-conductors on the interfacial electronic properties.

MINTWELD

Manufacturing industry, metal alloys, welding, EAM (electric active materials) modeling

MODIFY

Modelling has explained the interplay between the chemical composition of the synthesized PSA samples and the degree, strength and life-time of the specific hydrogen forces developing in the polymer, which in turn governs the unique cohesive properties and strong elasticity of these materials. Models also explained the big role played by particle-to-particle transient forces on the elasticity-to-viscosity ratio which seems to be at the heart of the design task for new adhesives. Modelling explained the connection between bulk rheological
properties in extension and shear and the debonding mechanisms during stretching of PSAs.

MONAMI

Modelling of materials properties allows the search for new materials or to make accurate interpretations of observed materials phenomena. An example can be found for magnetic materials where two properties are most important from an application point of view, namely the size of the saturation moment at room temperature and a large magnetic hardness (or synonymously, a large magnetic anisotropy energy – MAE). These two properties can be predicted for any material, with an accuracy that is needed to make the search for novel permanent magnetic materials much more efficient.

MORDRED

Predict defect character and density that causes device breakdown in realistic environments and over realistic performance times.
Characterize this for a variety of new, industrially untested materials.
Suggest routes for device design that should eliminate or reduce reliability problems

MULTIHY

Optimisation of the pulse-plating process used in the fabrication of the combustion chamber of the Ariane satellite delivery vehicle
Mechanistic understanding of the susceptibility of advanced high strength steels to HE by absorbed H
Prediction of the influence of H on the fatigue lifetime of wind turbine bearings.

MUST

The model can be used do give recommendation concerning optimal composition and structure of the coating to delay corrosion of metallic and polymeric substrates and structures, thus reducing development costs.
The model predicts service-life time via the probability of the scratch healing or inhibition based on the physico-chemical properties of the materials and realistic scratch geometries.

NAMASTE

Reproduction of the valence band nature of Fermi level states the archetypical ferromagnetic semiconductor (Ga,Mn)As. Prediction and explanation of the observed magnetic and magneto-

transport properties in ferromagnetic semiconductors.Understanding of the observed spin-torque effects which lead to the discovery of new ferromagnetic resonance (FMR) effects. Based on the developed capabilities to model spin-orbit in metals, it was shown that appropriate antiferromagnetic materials could be employed as active layers in spintronic devices (GMR, etc), thus opening up the possibility of the new field of antiferromagnetic spintronics.

NANOINTERFACE

A set of design and reliability guidelines guidelines for microelectronic packages for microelectronic packages with respect to delamination risk has been elaborated, which can only be generated in a systematic way by accurate models.
A better, quantitative understanding of adhesion mechanisms at the very small to macroscopic scale and of the effect of surface roughening on adhesion properties has been provided. This was only possible via meso-scale semi-analytical and numerical fracture mechanics models.

NANOMAGMA

The model predicted that the optical and magneto-optical response of complex structures where metals and magneto-optical materials are simultaneously present is proportional to the electromagnetic field in the magnetic material. This guided the design and now the whole structure is grown to try to maximize the field in that material.

NANOMODEL

The role of the interphase (structure and dynamics) is difficult to investigate experimentally. Only modelling can give access to the very structure of matrix, nanoparticles and their interphases. Modelling revealed details how the interface is influenced by the chemistry.

NIM_NIL

Modelling allowed the optical properties to be calculated before the sample is fabricated, being essential for design and leaving room for optimization. Once a sample is fabricated and characterized, modelling gave results usually in excellent agreement with measured data, allowing to understand the underlaying physics and proving the sample high quality. It helped identify the EM properties of fishnets in the wedge configuration demonstrating the operation of a metamaterial in the visible regime.

NPMIMETIC

The study of the intervertebral disc (IVD) mechanical behaviour presents a high level of difficulty, due to intrinsic uncertainty on the quantification of real working loads (coupling compression forces, flections and torsion moments). Post-mortem analysis doesn't allow a full understanding of these phenomena, mainly due to the highly hydrated nature and the fact that the osmotic role of nucleus function is not achieved in those conditions. Modelling can overcome these restrictions and predict two fundamental situations:

i) degenerated IVD – stress/strain conditions due to nucleus degeneration (geometry, stress conditions, prediction of overstretched annulus' fibres)
ii) restored IVD – prediction of restoration conditions, annulus rupture state and/or failure risks on the nucleus 'refilling' process, influence of nucleus prosthetic materials characteristics on overall mechanical stability

OXIDES

Theoretical predictions to be further validated experimentally:

The unexpected possibility to induce multiferroism in epitaxially strained $CaMnO_3$
The unexpected possibility to achieve exploitable Tunnel Electro-Resistance (TER) in symmetric Ferroelectric Tunnel Junction (FTJ); for memory applications
The prediction of the unexpected appearance of a half-metallic ferromagnetic highly-confined 2-dimensional electron gas (2DEG) in $SrTiO_3/SrRuO_3$ superlattices
The unexpected role of oxygen rotation in shifting by 300 K the ferroelectric phase transition of $PbTiO_3$;

Joined theoretical-experimental breakthroughs

Improper ferroelectricity in oxide superlattices in which modelling identified a new microscopic mechanism (the so-called trilinear coupling of structural instabilites) as observed in parallel experimentally
Exchange bias in $LaNiO_3/LaMnO_3$ superlattices; modelling allowed the proper understanding of the unusual spin order giving rise to the experimental results
Compelling evidence of the intrinsic nature of the 2DEG at polar oxide interfaces; modelling of ideal interfaces was required to unambiguously distinguish between intrinsic and extrinsic effects
Confinement properties of the 2DEG at the $LaAlO_3/SrTiO_3$ interface; modelling provides key information on the electronic band structure, mandatory to interprete measured properties

POCO

Molecular models of functionalized CNTs and polymer matrices could predict the influence of the functional groups on the mechanical properties of the CNT and the interfacial shear strength (IFSS) of the nanocomposites. The influence of the functionalization of CNTs on the IFSS of the nanocomposite was demonstrated, something that would otherwise have cost many experiments.
The pull-out of CNTs from molecular matrices is difficult to analyze by experimental methods due to the scales involved. In this case, the process modelling of the pull-out was necessary to analyze the interfacial shear strength of the nanocomposites.

RADINTERFACES

The modelling is going to guide the appropriate tuning of interfaces within multi-laminate composite materials to obtain defect absorption materials with a self-healing mechanism.

REFREEPERMAG

The theory can pre-identify interesting materials prior to the actual synthesis and experiments and thus save time and resources.

ROLICER

The FEM simulations provide solutions for material stresses, which cannot be obtained experimentally. The fracture models describe crack nucleation based on traction-separation laws which provide a phenomenological lifetime prediction tool without the need for extensive experiments.

The microscale models achieve homogenisation of thermoelastic properties and thermomechanical homogenisation of strengthening effects in ceramics. Such simulations provide information that cannot be obtained experimentally.

The ab initio models provide reliable properties of the bulk material and solid-solid interfaces as criteria for crack initiation, which are very difficult to obtain by experiments.

Molecular dynamics models are used in modelling hybrid steel-ceramic contact to study the interaction between additives in lubricants and bearing surfaces. Experiments that provide such information are not possible.

SIMBA

The modelling of the plasma flow dynamics and particle trajectories permitted to define the process at different scales and to predict the influences of the main process parameters (e.g. effects on nanopowder production yield when changing the reactor geometry and operating conditions).

The model enabled the design of an optimum reactor chamber with increased flow of particles for collection thus avoiding an expensive try-and-fail approach, and saving time and effort in optimising the lab scale process and in transferring main results to an industrial ICP installation.

SIMUGLAS

Shape of moulds can be now predicted with the help of modelling of the glass shrinkages, which had to be done previously by expensive try-out experiments.

Index drop inside glass lens can be now predicted with the help of modelling of the structure relaxation behaviour of glass material, which was unknown only by pure experiments.

Material flow and temperature during forming process can be predicted, which cannot be observed and measured in the real moulding process.

SMASH

The modelling and simulation of GaN-based LEDs is able to guide the device design, by optimizing strain, polarization and quantum effects in order to improve the performance of the devices. Atomistic simulations can shed light on the effect of clustering in the alloy active regions.

SSEEC

The materials modelling of the overall system gave us invaluable feedback on experimental development, reducing the time that would otherwise be required to make multiple measurements or a full phase space of physical samples.

The 2D model of an active magnetic regenerator (AMR) enabled accurate optimisation of geometry (packing density, absolute length scales), system operating parameters (frequency, flow rate) and identification of optimal (or ideal) refrigerant material properties (magnetocaloric effect and heat capacity) against overall efficiency and power requirements.

SUPER-IRON

Prediction of high-pressure phase transitions in $Ba(Ca)Fe_2As_2$ and of non-hydrostatic effect, confirmed by high-pressure XRD measurements.

Prediction of the peculiar structural and electronic modification upon doping with rare-earth metals in $CaFe_2As_2$.

Understanding of disorder, surface and interface effects.

Model calculations, joined with DFT calculations, were able to predict a tri-critical point in the phase diagram of iron-pnictides, now a hot subject for experimental confirmation.

SUPERLION

The model allowed shortened and better-informed selection of the most efficient cell architectures and geometries, and the optimal cell materials. Modelling can avoid excessive and often futile efforts to create more impressive micro-architectured electrodes, since these will often not result in improved battery performance.

SURFUNCELL

Modelling reproduced and predicted the strength and structured build-up of hydrogen bonds of water to the cellulose surface and inside the water layer as a function of the water layer thickness. This lead to suggestions for the design of the surface structure and charge distribution at cellulose surfaces.

ULTRAMAGNETRON

Materials with a compensation point are shown to be very promising media for magnetic recording. The magnetization reversal by a single circularly polarized laser pulse has been successfully simulated A phase diagram for opto-magnetic reversal was obtained, demonstrating a window of peak electron temperature and effective magnetic field pulse duration for opto-magnetic switching. A new mechanism of linear magnetization reversal was discovered. Experimentally the two sublattices of a ferrimagnetic alloy (GdFeCo) were found to demagnetise at different rates which was then confirmed by the model.The model predicted that the ferrimagnet transitioned into a transient ferromagnetic phase stable for only around 300femtoseconds which was found experimentally. The theoretical model predicted that the magnetisation of the ferrimagnet reversed spontaneously on application of a heat pulse, which was then experimentally verified.

Annex I
Projects fiches

The modelling done in some 50 materials projects in the NMP Programme is described in individual project fiches. The past tense is used for projects that have finished at the time of writing (summer 2012) and the present tense for projects still on-going.
To show the value of modelling, the achievements of the models beyond experiments have been listed. Text in the fiches describing developments of models and constitutive equations are highlighted in yellow.

Modelling

in ADGLASS 229205

Subject of the modelling
Protein adhesion, interface cohesion and crack propagation in glasses

Models used

Atomistic MD and QM/MM (with extended buffer zone to mitigate the effects of its artificial surface)

Simulation software and type of numerics used
QUIP, CP2K, Amber, with ad-hoc modifications
Plug-ins for other academic/industrial codes (e.g. LAMMPS, OpenKIM, VASP, Castep)

Achievements of the model beyond experiments
The modelling revealed previously unknown details of an important process (hydrogen embrittlement of silicon crystals) widely employed for the fabrication of Silicon-On-Insulators (SOI) nanoelectronic devices. It also unveiled undiscovered mechanisms of brittle fracture in solid materials, including the precise chemomechanical role of defects (impurities, reconstructions, dislocations) and dynamical instabilities during the propagation of cracks in brittle materials. Moreover, the simulations explained the reasons for the previously observed, yet so far very poorly understood, binding specificity of certain peptide sequences to inorganic materials surfaces. They revealed an unknown adhesion driving force modulated by the local variations of water density at the solid/liquid interface.

Application
Pharmaceutical and biomedical products
Optical and photovoltaic devices
Architectural panels

Relevant review articles
J. Schneider, L. Colombi Ciacchi, “Specific material recognition by small peptides is mediated by the interfacial solvent structure”, Journal of the American Chemical Society 134, 2407-2413 (2012)
N. Bernstein, et al “QM/MM simulation of liquid water with an adaptive quantum region”, Physical Chemistry Chemical Physics 14, 646-656 (2012)
F. Atrash and D. Sherman, “Dynamic Fracture Instabilities Generated by Phonon Emission: Experiments and Atomistic Simulations”, Journal of the Mechanics and Physics of Solids 60, 844-856 (2012)
G. Moras, et al “Atomically smooth stress-corrosion cleavage of a hydrogen-implanted crystal”, Physical Review Letters 105, 075502 (2010) (Featured in Physical Review Focus, vol. 26, 13th August 2010)

Summary of the project

The project target detailed knowledge of chemical and physical processes taking place at glassy interface systems and is devoted to improving the efficiency, functionality and reliability of glass products for pharmaceutical and photovoltaic applications.

Summary of the modelling

The project applied multi-scale hybrid quantum-mechanical (QM/MM), atomistic modelling methods. Large length scales (many tens of thousands of atoms) are required to describe the systems of interest, and key physics have been added in quantum mechanical models, combining the highly accurate QM models with the fast MM dynamics.
The QM calculations are performed on a limited portion of the system which includes an extended buffer zone to mitigate the effects of its artificial surface. The QM calculations are only carried out when the dynamic evolution of the system leads it out of the range of configurations which can be accurately simulated by the classical potential alone (e.g. during chemical reactions involving bond breaking or forming).
This method is applied for example to the simulation of fracture experiments where the mismatch between the thermal expansion coefficients of frame and specimen generate normal and tangential strain fields at the specimen's boundaries that serve as the driving force for crack initiation and propagation.
We have extended the method so that it can handle liquids, which enables us to study solid/liquid interfaces.
The novel method has been applied to two scientific problems which require at the same time quantum precision and very large model system sizes. Namely, we have investigated (i) the adhesion of proteins at the interface between a glassy SiO_2 phase and a water solution, relevant to pharmaceutical applications and (ii) the cohesion between heterogeneous glassy interfaces (e.g. containing SiO_2 and TiO_2 phases) relevant to thin-layer-based conditioning of glass materials for applications in architectural glass and photovoltaic cells.
To aid the above applications, the electronic degrees of freedom from an explicit quantum mechanical model have been removed without sacrificing the accuracy of the atomistic potential, formally derived from quantum mechanical models. We gain speeds of many orders of magnitude. Novel quantum-accurate classical potentials have been created for carbon, silicon, water, tungsten, and various oxides.

www.adglass.eu

Project Acronym and Number: ADGLASS 229205
Project Title: Adhesion and Cohesion at Interfaces in High Performance Glassy Systems
Start and End Dates: 01/01/09/2009 till 28/02/2013
EU Contribution: 2.999.622 €
Coordinator: Lucio Colombi Ciacchi, University of Bremen and Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Bremen, Germany,colombi@hmi.uni-bremen.de

Modelling

in AMCOS 233502

Subject of the modelling
Zeolitic imidazolate frameworks, hyperbranched aminosilicas, functionalised polymers: advanced materials for selective sorption of carbon dioxide from gaseous mixtures.

Models used
Density Functional Theory (DFT) for electronic structure calculations
Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) approaches.
Statistical mechanics-based molecular simulation methods (Metropolis Monte Carlo in the grand canonical ensemble, molecular dynamics, dynamically corrected transition-state theory)
Statistical mesoscopic flow simulation methods (Kinetic Monte Carlo, Lattice Gas Cellular Automata)

Simulation software and type of numerics used
Numerical solution of initial value problems in ~105 unknown functions of time.
Stochastic sampling of multidimensional spaces spanned by ~105 coordinates according to prescribed probability density functions.
Computation of minima and saddle points on complex potential energy hypersurfaces of the high dimensionality stated above.

Achievements of the model beyond experiments
Simulations can predict the sorption isotherms of pure and mixed gases in recently synthesized nanoporous materials (zeolites, metal-organic frameworks, polymers), or in hypothetical materials considered for synthesis. They can also predict the rates of diffusive transport through these materials.

Application
Capture of CO_2 released from industrial processes and for industrial gas separations.

Relevant review articles: Pantatosaki, E.; Pazzona, F.G.; Megariotis, G.; Papadopoulos, G.K. "Atomistic Simulation Studies on the Dynamics and Thermodynamics of Nonpolar Molecules within the Zeolite Imidazolate Framework-8", J. Phys. Chem. B 2010, 114, 2493-2503.
Jobic, H.; Theodorou, D.N. "Quasi-elastic neutron scattering and molecular dynamics simulation as complementary techniques for studying diffusion in zeolites", Microp. Mesop. Mater. 2007, 102, 21-50

Summary of project

The objective of the EU-India collaborative research project AMCOS is to investigate newly synthesized and/or modified classes of advanced sorbents, such as the zeolitic imidazolate frameworks (ZIF), functionalized polymers (FP), and the new category of inorganic-organic hybrid sorbents known as hyperbranched aminosilicas (HAS). Thanks to their exceptional physicochemical properties and enhanced ability for adsorbing specific groups of molecules, these advanced materials have been used for environmental and energy-related applications, such as the selective separation of carbon dioxide from flue gases and natural gas. Aiming at a rational materials selection and optimisation strategy for these applications, the sorbate molecular dynamics and thermodynamics in these materials are studied extensively by applying, developing and integrating state-of-the-art computational tools and experimental methodologies.

Summary of the modelling

Computer modelling has been utilized mainly for the study of CO_2-sorbent interactions along with the mobility of a wider class of guest molecules in the various advanced materials host systems, such as hyperbranched aminosilica (HAS), zeolitic imidazolate frameworks (ZIFs), and functionalised polymers. A focus of the project is the selective separation of CO_2 from CO_2/CH_4 and CO_2/N_2 mixtures, which is important for CO_2 capture and CH_4 enrichment, respectively, for environmental and energy resource related applications.
The ZIF-8 crystal was modelled using rigid and flexible models, starting from conventional general-purpose force fields (Dreiding) and proceeding to more refined energy expressions that better represent specific interactions with the metal atoms. Quantum mechanical calculations have provided a new, more reliable input for the values of the partial charges of the ZIF framework atoms. DFT calculations on periodic structures were performed using BLYP and PBE functionals. We have found that the fluctuations of the atomic charges are almost negligible, hinting that using a simple point charge approximation for classical Molecular Dynamics simulations of ZIF-8 is sensible. We have also applied an ab initio quantum mechanical model to calculate the force field of the ZIF-8.
Using these improved tools for describing interactions, we have designed and implemented efficient grand canonical Monte Carlo and molecular dynamics simulations for predicting the sorption isotherms (equilibrium amount of gas sorbed per unit mass of nanoporous material at given temperature and pressure) and diffusivities of hydrogen (H_2), methane (CH_4), and carbon dioxide (CO_2) in the project materials. Predictions are generally in very good agreement with the measurements conducted by the experimental partners of the project, validating our predictive computational approach.

http://comse.chemeng.ntua.gr/amcos/

Project Acronym and Number: AMCOS 233502
Project Title: Advanced Materials as CO2 Removers: A Computational Study of CO2 Sorption Thermodynamics and Kinetics
Start and End Dates: 01/05/2009 till 30/04/2012
EU Contribution: 520.000 €
Coordinator: Doros Nicolas Theodorou, National Technical University of Athens, GR doros@central.ntua.gr

Modelling

in AMON-RA 214814

Subject of the modelling
III-V Semiconductor materials, devices and systems

Models used
Electronic models: drift-diffusion, linear continuum mechanics for strain, k.p theory for band structure calculation
Optical modelling (ab-initio) finite-element method for vectorial Maxwell equations

Simulation software and type of numerics used
Electronic models
- EtaOpt (used)
- Sentaurus Device (DESSIS) (used)
- QUATRA/CELS (used and developed)

Optical modelling (ab-initio)
- Fdmax (formerly lumi3) (used and developed)
- EtaOpt (used)
- Scattering MatrixMEthod (used and developed)

3-dimensional vectorial finite-element method for eigenproblems extended to model scattering problems on general unstructured meshes, Maxwell equations, Drift-Diffusion equations

Achievements of the model beyond experiments
The model guides device development by
Definition of suitable bandgap energies for single- and dual-junction nanowire solar cells
Definition of suitable device structure including doping levels and barrier layers
Definition of optimum configuration for wire length, distance and diameter in nanowire array
Understanding of optical and electrical loss mechanism in single- and dual-junction nanowire solar cells
Contribution to roadmap for assessment of III-V nanowire photovoltaics

Application
IIIrd Generation Photovoltaics
Solar Cells
Nanowire Optoelectronics

Relevant review articles
J. Kupec, B. Witzigmann, 'Computational electromagnetics for nanostructured solar cells', J. Comp. El., 2012, invited review
B. Witzigmann, R. Veprek, S. Steiger, and J. Kupec, 'Comprehensive Modeling of Optoelectronic Nanostructures', J. Comp. El., No. 4, Vol. 4, pp. 389-397, 2009, invited reviewstress-corrosion cleavage of a hydrogen-implanted crystal", Physical Review Letters 105, 075502 (2010) (Featured in Physical Review Focus, vol. 26, 13th August 2010).

Summary of the project

The project AMON-RA targeted photovoltaic cells made from arrays of light-harvesting nanowires on silicon substrates made with hetero-epitaxy of III–V semiconductors. Two main architectures were investigated: The first, called “Light Guiding made from core-shell nanowires, in which the sunlight will be guided through materials with decreasing band gap. The second architecture, called “Effective Medium”, consists of denser arrays of much thinner wires, where the light waves will experience an effectively averaged medium as they propagate downwards. The high degree of self-assembly and insensitivity to lattice parameters and the use of inexpensive silicon substrates made the production cheap.

Summary of the modelling

The optical and electronic properties of nanowire photovoltaic cells are modeled using existing multi-dimensional simulation methods. In addition models combining optoelectronic and quantization effects in a heterojunction nanowire were developed within AMON-RA.
A simple program EtaOpt evaluates the optimum bandgap combination for multi-junction solar cells with two or more junctions depending on the spectral conditions and calculates the thermodynamic efficiency limit for a given bandgap combination.
The optical properties of nanowire arrays are modelled solving Maxwells equations with a 3-dimensional finite element method or a scattering matrix method.
A model within CELS/QUATRA for optical carrier generation in nano-wires including excitonic and phonon loss effects (optical absorption) is derived and implemented. It is based on the semi-classical drift-diffusion method (second principle). The electronic simulation of carrier transport in large diameter hetero-junction nanowires with tunnel junctions is described with multi-scale semi-classical and quantum-mechanical methods.
A detailed analysis of current flow and resistance is performed, and the optimum wire configuration is determined. The electrical modeling of the Esaki interband tunneling diode the most critical part of the solar cell, is done by the commercial DESSIS software.
(A coupled opto-electronic model for a heterojunction nanowire, including quantization effects is used within AMON-RA.)
In summary, modeling in AMON-RA focuses on the customization of existing models and numerics for nano-wires, and their application to nano-wire design for photovoltaics.

www.amonra.eu

Project Acronym and Number: AMON-RA 214814
Project Title: Architectures, Materials, and One-dimensional Nanowires for Photovoltaics - Research and Applications
Start and End Dates: 01/10/2008 till 30/09/2012
EU Contribution: 3.199.987 €
Coordinator: Prof. Knut Deppert, Lund University, knut.deppert@ftf.lth.se

Modelling

in ARTIVASC_3D 263416

Subject of the modelling

Blood and nutrient transport in vascularised biomaterials

Models used

Hydrodynamics model based on Navier-Stokes equations
Transport model based on advection-diffusion equation

Simulation software and type of numerics used

Finite Element (FE) software
Smoothed Particle Hydrodynamics (SPH) software

Achievements of the model beyond experiments

The hydrodynamic modelling will be able to predict wall shear stresses at the vascular graft walls. These stresses have to be within a certain range in order to stimulate the endothelial cells to perform e.g. neo-angiogenesis.. These wall shear stresses would be extremely difficult to measure for any possible graft geometry. Therefore, a modelling-based design approach is crucial for tissue engineering.

Application

Regenerative medicine, additive manufacturing

Summary of project

ArtiVasc 3D aims at developing a bioartificial vascularised skin which will, for the first time, allow tissue replacement with optimum properties in a fully automated and standardised manufacturing approach. This will be achieved through an innovative combination of hi-tech engineering such as micro-scale printing, nano-scale multiphoton polymerisation and electro-spinning with biological research on biochemical surface modification and complex cell culture and using a multidisciplinary approach which involves experts in biomaterial development, cell-matrix interaction, angiogenesis, tissue engineering, simulation, design and fabrication methods work.
This new bioartificial vascularised skin will be of great value in a vast array of clinical treatments, e.g. as a transplant in trauma treatment. In addition, it will be used as an innovative in vitro skin equivalent for pharmaceutical, cosmetics or chemical substance testing, which represents a promising method to reduce expensive, ethically disputed animal testing.

Summary of the modelling

The project develops and applies modelling techniques for the design a vascular system that effectively delivers O_2 and other nutrients from the circulating blood flow to the surrounding tissue. Experiments and simulations will be employed in order to develop design rules and 3D models of the artificial vascular system. The modelling in this project aims at providing the link between biological demands and the scaffold manufacturing and development.

An advection-diffusion model is applied to predict permeation times of nutrients and O_2 depending on material type (e.g. polymer, hydrogel, fat), and vascular system parameters like porosity and wall thickness. The simulation model explicitly considers the local porosity structure and, thus, gives far more detailed results than simple calculations using Darcy's Law. Model parameters will be adjusted by reference to the experimental data. The model is used to calculate permeation times which are necessary for the nutrients/O_2 to reach the cells in the surrounding hydrogel matrix.

The avoidance of clogging of the vascular grafts is of paramount importance to the long-term functionality of the system. In order to account for this aspect, the smoothed particle hydrodynamics solver will be extended by a deposition model. This allows for the analysis of deposition of platelets on the vessel walls depending on systematically varied flow conditions. Based on these microscopic simulations deposition/clogging rules will be derived to be incorporate into the finite element modelling on the length-scale of the complete vascular system.

Fluid dynamics simulations of pulsatile blood flow through elastic blood vessels will be conducted and compared with pressure-controlled experiments. For this purpose a fluid-structure-interaction scheme will be used within the hydrodynamics code.
The blood flow simulations will provide information on the local geometry. Design rules for the local geometry (e.g. bifurcations, diminutions) will be derived. These rules will ensure the avoidance of flow anomalies (recirculating flows) and the compliance with a reasonable range of wall shear stresses to provide an endothelium-friendly flow environment. Thereby, neo-angiogenesis will be stimulated and clogging of the vascular grafts will be avoided.
The numerical results will be used for the 3D design of the complete artificial vascular system. The modelling-based design will ensure biomimetic conditions for the endothelial cell layer which is the key to a functional vascularised system.

http://www.artivasc.eu/

Project Acronym and Number: ARTIVASC_3D 263416
Project Title: Artificial vascularised scaffolds for 3D-tissue-regeneration
Start and End Dates: 01/11/2011 till 31/10/2015
EU Contribution: 7.800.000 €
Coordinator: Arnold Gillner, FhG, DE Arnold.Gillner@ilt.fraunhofer.de

Modelling

in ATHENA 233553

Subject of the modelling

Transition metal oxides (magnetic perovskites, double perovskites, diluted magnetic ferroelectrics, piezoelectrics, magneto resistivity heterojunctions, superlattices and multilayers)

Models used

First-principles density-functional theory (DFT) based methods.
Tight binding model.

Simulation software and type of numerics used

High performance electronic structure codes based on density functional theory: highly parallelised versions of the LCAO-based SIESTA code, the PWSIC code, the developer version of VASP. Model Hamiltonian solved with a range on Monte Carlo technique, including the travelling cluster scheme for large-scale simulations.
Maximally localized Wannier function suit WanT, interfaced with the DFT codes to give parameters for the model Hamiltonian
The integrated multi-scale approach (DFT WanT MH) allows a full parameter-free description of thermodynamics properties of complex oxides and oxides interfaces ahead of experiments, or where experimental information are difficult/impossible to extract.

Achievements of the model beyond experiments

Identification of candidate materials and materials interfaces for future nano-electronics based on complex oxides. These included hetero-junctions, superlattices and multilayers consisting of doped magnetic perovskites (e.g. LaxSr1-xMnO3, PrxCa1-xMnO3), double perovskites (e.g. LaNi1-xMnxO3) and diluted magnetic ferroelectrics designed to exploit and manipulate the coupling of different order parameters at the two sides of the interface.
Prediction of the phase diagram of complex magnetic oxides MnO and NiO under pressure,
Explanation of the extremely high antiferromagnetic ordering temperature in SrTcO3 and BaTcO3,

Application

Multiferroic devices (both single-phased multi-functional materials and heterostructures), non-volatile memories based on multiferroic materials

Relevant review articles

A. Filippetti, et al Variational pseudo-self-interaction-corrected density functional approach to the ab initio description of correlated solids and molecules, Phys. Rev. B 84, 195127 (2011).
T. Archer, et.al Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods, Phys. Rev. B 84, 115114 (2011).
C. Franchini, et al. Exceptionally strong magnetism in the 4d perovskites RTcO3 (R=Ca, Sr, Ba), Phys. Rev. B 83, 220402(R) (2011).

Summary of project

The overall aim of the project is the investigation of the properties and functionalities of transition metal oxides and their heterostructure, as these may be viable candidates as building blocks of future micro- and nanoelectronic devices. The project investigates the physics of strong-correlated materials, which includes charge and orbital ordering, polaronic formation, spin-charge separation, non-Fermi liquid behaviour, just to name a few.

Summary of the modelling

The modelling consists of a multi-scale approach merging parameter-free first-principles methods based on density-functional theory (DFT) with many-body model Hamiltonian calculations suited for exploring the thermodynamic properties of strong-correlated systems. On the one hand, first principles techniques allow one to describe at a quantitative level the electronic structure of perfectly crystalline materials at zero-temperature. In this case the description does not necessitate parameters as the underlying quantum mechanical problem is solved exactly, within well-controlled approximations. On the other hand, the model Hamiltonian approach is suitable for exploring effects connected to finite temperature and disorder. This however requires parameters, which usually are extracted from experiments, whenever possible, or simply inferred from chemical/physical intuition. Our research strategy combines the benefits of the two approaches as the parameters for the model Hamiltonians are rigorously extracted from our first principles calculations.

The project developed several methodologies for first principles calculations tailored to the specific class of materials comprising complex oxides and their interfaces and heterojunctions. This is a class of materials critical to standard electronic structure methods, which usually fail in describing even the most elementary properties as the electronic band-gap or are too expensive to use for interfaces. Our newly developed methods are based on DFT and include a completely novel variational formulation of the pseudo-self-interaction correction scheme (pSIC), a new version of the DFT exact exchange method, the hybrid Hartree-Fock DFT approach and a hybrid method combining DFT with the dynamical mean-field scheme.

The project formulated novel model Hamiltonians for describing the finite-temperature thermodynamic properties of single and double perovskites, with the possibility of including both A- and B-site doping/disorder. The parameters for the models are rigorously derived by a procedure in which the DFT-calculated electronic band-structure is mapped onto a tight-binding model. Such a mapping is carried out by constructing the system's maximally localized Wannier function, which is a universal procedure applicable to any material, no matter its complexity. New interfaces between the consortium available first principles codes (SIESTA, VASP and PWSIC) and the maximally localized Wannier function suit (WanT) have been constructed and will be soon distributed.

Achievements of the project include 1) the description of the phase diagram of both MnO and NiO under pressure, 2) the explanation of the spectacularly high antiferromagnetic ordering temperature in SrTcO3 and BaTcO3, currently the two materials with the highest Neel temperature among the 4d series, 3) the demonstration of the possibility of the coexistence of a tunnelling magneto-resistance and tunnelling electro-resistance in a complex oxides heterojunction, SrRuO3/BaTiO3/SrRuO3, and the tuning of the effect by intercalating a think SrTiO3 layers at one of the junction interfaces. 4)The project designed a new heterojunction stack, SrRuO3/BaTiO3/SrTiO3/SrRuO3, displaying both tunnelling magnetoresistance (TMR) and tunnelling electroresistance (TER). Furthermore we demonstrated that the TER is fully tuneable by changing the SrTiO3 layer thickness. This may have significant application as a 4-state non-volatile multifunctional random access memory element. Predictions on new devices functionalities are now possible.

www.athenacomp.eu

Project Acronym and Number: ATHENA 233553
Project Title: Advanced theories for functional oxides: new routes to handle the devices of the future
Start and End Dates: 01/06/2009 till 31/05/2012
EU Contribution: 849.998 €
Coordinator: Stefano Sanvito, Trinity College Dublin, Ireland, sanvitos@tcd.ie

Modelling

in AUTOSUPERCAP 266097

Subject of the modelling

Battery-supercapacitor power system for an electric vehicle (EV) application
Ion transport in supercapacitors made of carbonaceous materials, e.g. activated carbon, carbon nanotubes, graphene

Models used

Classical MD code for ion transport model electrolyte transport and the minimum electrode pore size required
Device model for optimal control of a battery-supercapacitors systems

Simulation software and type of numerics used

Matlab Simulink for power system
Materials Studio v5.0 for molecular ion simulations

Achievements of the model beyond experiments

The battery-supercapacitor modelling and simulations allow selection of the best materials/supercapacitor for scaling up reducing experimental costs.
The molecular ion simulations guided the research for a pore size, maximising the specific capacitance for carbonaceous electrode materials and thereby increasing energy and power density.

Application

supercapacitors for energy storage units

Relevant review articles:

A. Santucci, F. Markoulidis, M.K. Abbas, C. Lekakou, B. Martorana, M. Gosso and J. Perry “A Model of a Battery-Supercapacitor Power and Energy Storage System for Electric Vehicle Applications”, submitted to International Journal of Powertrains, May 2012
C.Lekakou, F.Markoulidis, C.Lei, A.Sorniotti, J.Perry, C.Hoy, B.Martorana, I.Cannavaro, M.Gosso “Meso-nano and micro-nano ion transport in porous carbon composite electrodes for energy storage applications”, Proceedings ECCM15 - 15TH European Conference on composite materials, Venice, Italy, 24-28 June 2012

Summary of project

The project is aiming at developing supercapacitors which are essential in electric vehicles for supplying power during acceleration and recovering braking energy. High power and high energy density are required in the automotive industry for both an effective power system but also to reduce weight.

Summary of the modelling

The project works with computer simulations to optimise the power system and the design of supercapacitor banks. An existing generic power system and electric vehicle computer model have been elaborated with a model for a battery-supercapacitor energy storage unit (ESU) or a battery only ESU. Input to the model is imposed driving time schedule, in terms of speed and requested power as functions of time, imposes power requirements to a dc bus and associated control system. charge cycles will also be incorporated in the model as a control sub-loop, including charging of supercapacitor and battery from combined energy sources, e.g. fuel cell, electricity sub-stations, braking energy during the deceleration phases of the driving schedule. The fast discharge and charge phases impose a requirement for reliable and optimum operation, especially in urban driving schedules. The computer code to simulate these processes will be produced in MATLAB Simulink environment.
This power system computer model has been incorporated in the test rig computer model and in a generic electric-hybrid vehicle model (for parametric studies) to decide on the specifications of a generic electric-hybrid vehicle model. With this model, parametric and optimisation studies will be carried out for different scenarios in automotive applications and different battery-supercapacitor load combinations in order to establish supercapacitor specifications for the different types of supercapacitors to be developed in this project.
The work will aim to establish the 'real world' working envelope of typical supercapacitor energy storage systems. This will lead to minimisation of system mass, a very important consideration for an electrical vehicle, and also the cost of the system.

The project also develops classical molecular dynamics model for ion transport to design and tailor optimum electrode material morphologies for the ion transport of certain electrolytes to achieve maximum power and energy densities.
In energy storage devices carbonaceous composite electrodes are a popular choice, consisting of activated carbon (ac), conductive additives and a polymeric binder matrix. The active electrode components are in the form of ac particles, ac fibres, or ac monolith combined with conductive additives such as carbon black. Activated carbon plays the most important role for storing a large amount of energy in the form of ions contained in the carbon nanopores. This study considers a modelling approach to the meso-nano and micro-nano infiltration of ions into the porous carbon structure during the operation of the energy storage device. Depending on the pore size, ion size and solvent molecule size, ions may be solvated or unsolvated as they move, where ions are solvated in meso-pores for most cases. Molecular model simulations (Materials Studio v5.0) have been performed to determine the values of the geometrical parameters of different ions, solvated and unsolvated in various solvents. A meso-nano and micro-nano ion infiltration model has been developed in this project under both steady state and dynamic conditions. The model is going to be implemented into a computer code and it will be run for various input parameters to optimise speed, extent of ion transport and capacitance in a porous material.

http://autosupercap.eps.surrey.ac.uk/

Project Acronym and Number: AUTOSUPERCAP 266097
Project Title: development of high energy/power density supercapacitors for automotive applications
Start and End Dates: 01/1/2011 till 31/12/2013
EU Contribution: 3.974.595€
Coordinator: Dr Constantina Lekakou, University of Surrey, UK, C.Lekakou@surrey.ac.uk

Modelling

in CODICE 214030

Subject of the modelling

Cement, cement hydration

Models used

Molecular Dynamics (Garofalini force field) for hydration
Hierarchical Monte Carlo growth model for aggregation of C-S-H particles
Grain-based flow, chemistry and mechanical model for hydration (extended Nerst-Planck equations)
wear and fracture model

Simulation software and type of numerics used

HYMOSTRUC-3D for hydration
CODICE_HYD Monte Carlo growth model (based on C4)
CODICE_DEG and CODICE_MEC for wear and fracture (Finite Elements)

Achievements of the model beyond experiments

The developed toolkits revealed that there is a synergy in the hydration of alite and belite phases of cement clinker, which opens the door to new eco-cements.
While a priori one would expect that the larger the content of C_3S the better the resulting mechanical properties, the simulations have revealed that there is synergy in the hydration of C_3S and C_2S blends, and that there is an optimum C_3S/C_2S ratio around 70/30.

Application

Eco cement for construction

Relevant review articles

Puertas F et al. A model for the C-A-S-H gel formed in alkali-activated slag cements; JOURNAL OF THE EUROPEAN CERAMIC SOCIETY Volume: 31 Issue: 12 Pages: 2043-2056 DOI:10.1016/j.jeurceramsoc.2011.04.036 Published: OCT 15 2011 –
Dolado Jorge S.; van Breugel Klaas; Recent advances in modeling for cementitious materials; CEMENT AND CONCRETE RESEARCH Volume: 41 Issue: 7 Special Issue: SI Pages: 711-726 DOI: 10.1016/j.cemconres.2011.03.014 Published: JUL 2011

Summary of project

CODICE brought producers and suppliers of cement-based materials together with universities and research institutes for the development of new and radically improved computational toolkits that monitor the formation and properties of cementitious materiales by starting from macroscopic processing variables: size of cement grains, water-cement ratio, temperature, grain composition.

Summary of the modelling

CODICE project has developed a serial parameter-passing multi-scale modelling scheme to predict the structural evolution and the mechanical performance of non-degraded and degraded cementitious matrices as a function of macroscopical processing variables to guide the design of cementitious materials in which the high density-C-S-H forms (high resistance to degradation processes) are promoted against the low density- C-S-H ones (low resistance to degradation processes), paying attention to the structure and processes occurring at the nanoscale which are crucial for the formation and properties of C-S-H gel (the most important ingredient of cement-based materials).

A1) Coarse macrolevel description in CODICE_HYD TOOLKIT

The coarser description of the cementitious skeletons is provided by a new and modified version of HYMOSTRUC-3D which is based on a mass balance concept for individual hydrating cement grains and distinguishes three independent phases, i.e. C3S, C2S and CH (E. A. B. Koenders et al.; A Density Model for Micro- to Nano-structures; under review). Moreover a novel digitalization mode has been implemented that generates a 3D voxel structure of the virtual microstructure and can be used for information exchange within the run of each time step. This new HYMOSTRUC-3D model employs as input macroscopical processing variables, such as the cement grain size, the water/cement ratio, etc and gives for each voxel relevant information like density, relative humidity, saturation, chemistry, etc.

A2) Refined nano-level description in CODICE_HYD TOOLKIT

The refinement of the coarse microstructure is performed by a Monte Carlo based algorithm named C4 (CODICE_Colloidal_CSH_Code) model. With the data flushed from the micro level simulations, each voxel can be refined. To this end, current implementation of C4 receives as input the density of the C-S-H voxel, and its water content (saturation index). Then the structure at the submicro level is conceived as a resulting from aggregation of dried C-S-H particles. The information about the size, density or water content of these basic dried-C-S-H units is based on the knowledge gained from intensive atomistic simulations. Afterwards the voxel structure is generated through Monte Carlo growth scheme which mimics the textural details provided by Jenning's model. This is possible by adjusting the growth parameters so as to reproduce the right density of the voxel, and the saturation index.

B) CODICE_DEG TOOLKIT simulates the accelerated degradation processes that occur when ammonium nitrate (NH_4NO_3) solutions pass into the cementitious pore network. In essence, it solves by standard Finite Element Model (FEM) the extended Nerst-Plank set of equations by decoupling the transport and chemical reaction equations. Remarkably, CODICE_DEG is well suited to trace the degradation processes at the C-S-H level, and to the best of our knowledge, it is the first time that the calcium leaching can be visualized in 3D. This new tools will contribute not only to a better understanding of the phenomenon of calcium leaching but they will also help engineers to the design of safer structures with smaller amount of material.

C) CODICE_MEC TOOLKIT, a 3D lattice fracture model, completes the "structure-performance" linkage by predicting the elastic modulus and tensile strength of cementitious skeletons starting from the knowledge of their structure. Finally, the outputs of the fracture process simulation are the load-displacement diagram and micro-crack propagation. The load-displacement diagram reveals the tensile behaviour of cement paste at micro-scale, from which the elastic modulus and tensile strength can be obtained.

www.codice-project.eu

Project Acronym and Number: CODICE 214030
Project Title: COmputationally Driven design of Innovative CEment-based materials
Start and End Dates: 01/09/2008 till 31/08/2011
EU Contribution: 2.700.000€
Coordinator: Jorge Sánchez Dolado, TECNALIA , jorge.dolado@tecnalia.com

Modelling

in CRONOS 280879

Subject of the modelling

Energy photo-conversion and laser-induced ultrafast magnetization dynamics

Models used

Full first principles method: time-dependent density functional theory (TDDFT)

Simulation software and type of numerics used

Open-source OCTOPUS code
OCTOPUS has a modular structure with a real-space grid as basis set.
Extreme parallelization with sparse matrix linear algebra

Achievements of the model beyond experiments

Prediction of full time-evolution of ultrafast pump-probe dynamics and their spectroscopy measurements for new materials. Prediction of charge oscillations in the electron transfer process in supra-molecular light harvesting organic triads. Prediction of demagnetization and spin-dynamics in bulk Ni in the first few fs subsequent an intense laser irradiation.

Application

Solar cell, magnetic recording

Relevant Review Articles

Time dependent DFT (the main theoretical tool of the project)
Miguel A. L. Marques and E. K. U. Gross, Time-dependent Density Functional Theory, Annual Review of Physical Chemistry 55, 427 (2004)

Dye sensitized solar cells
Anders Hagfeldt, Gerrit Boschloo, Licheng Sun, Lars Kloo and Henrik Pettersson, Dye-Sensitized Solar Cells, Chem. Rev. 110, 6595 (2010)

Ultrafast spin dynamics
Andrei Kirilyuk, Alexey V. Kimel and Theo Rasing, Ultrafast optical manipulation of magnetic order, Rev. Mod. Phys. 82, 2731 (2010)

Summary of project

The CRONOS project will go beyond the “static total-energy and mapping” scheme for materials modelling and develop a full time-dependent, fully atomistic theory of ultrafast dynamics in materials. The processes addressed are energy photo-conversion and laser-induced ultrafast magnetization dynamics.

Summary of the modelling

Photo-energy conversion and laser-induced ultrafast magnetisation dynamics both consist of describing how an electronic system reaches equilibrium after an initial perturbation pumps energy into it. This is governed by dynamics of materials at the femtosecond (fs, 1 fs=10-15 seconds) timescale and at the microscopic level. The modelling will address how the relaxation to the equilibrium can be driven towards a particular “useful” final state (for instance the separation of an electron-hole pair in a solar cell or the magnetisation reversal in magnetic recording).

Such dynamics are the result of the interplay between all the degrees of freedom involved, namely electronic, ionic and spin. Each one of them is characterised by a different timescale and by a characteristic interaction with the others. Furthermore the same degrees of freedom may evolve rather differently in different materials, so that fully atomistic modelling in the time-domain is necessary.

Time-dependent Density Functional Theory (TDDFT) will be the common theoretical/computational framework of the project. CRONOS will contribute to the development of TDDFT along four directions:

1) Development of new DFT and TDDFT meta-GGA exchange and correlation functionals
2) Development of new spin non-collinear DFT and TDDFT exchange and correlation functionals
3) Development of method to combine non-adiabatic ionic dynamics with time-dependent DFT
4) Development of optimal quantum control theory for TDDFT

The model will be parallelised so to ensure efficient scaling with system size.

Project Acronym and Number: CRONOS 280879
Project Title: Time dynamics and control in nanostructures for magnetic recording and energy applications
Start and End Dates: 01/06/2012 till 30/06/2015
EU Contribution: 3.380.058 €
Coordinator: Stefano Sanvito, TCD, Ireland, sanvitos@tcd.ie

Modelling

in DISC REGENERATION 213904

Subject of the modelling

Biomaterials, scaffolds, intervertebral disc, angiogenesis

Models used

Poroelastic model
Transport model

Simulation software and type of numerics used

Commercial software (Abaqus) with specific Fortran subroutines for non-linear material properties and coupling between diffusion, convection and structural analyses
Finite Element method with an implicit scheme
Parallelization for such non-linear model and such coupling between structural equations and thermodynamic equations

Achievements of the model beyond experiments

The modelling contributions are twofold:

- The coupled transport-mechano model is able to predict the movement of solutes within the intervertebral disc and predicts the interactions between mechanical properties, fluid and solute transport, and cell viability. This is essential for a proper understanding of the mechanisms of disc degeneration and disc regeneration with the use of biomaterials as disc substitute.
- Simulations of the effect of partial and complete disc nuleotomy on load transfer as a function of the biomaterial substitute used can be used to determine the surgical variability during nucleus removal.

Both contributions cannot be obtained experimentally and therefore are complementary to the experimental evaluation of the biomaterial performance.

Application

Bio medical implants

Summary of the project

The project seeks to provide a cure for lower back pain by developing injectable a-cellular and cell-loaded bioactive polymer-based scaffolds and technology which will repair a damaged intervertebral disc (IVD) by enabling its regeneration to a natural healthy state or better.

Summary of the modelling

This new generation of replacement devices are designed with a biomimetic approach which will confer the appropriate mechanical and biological properties and enable the inclusion of the requisite cell signalling factors to produce a bio-hybrid structure which closely resembles the human tissue in all its essential attributes.
This requires comprehensive numerical studies to predict their behavior under stress in the post-implantation period. Particular attention needs also to be paid to angiogenesis because in IVD tissue, vascularization must be carefully controlled, due to the unique anatomy and physiology of the intervertebral disc. Modelling studies within this project identified the key physical and mechanical properties of the natural IVD and the substitute materials, and provided an understanding of the physical aspects of the regeneration process.

1) Mechanical model

Complex computational models are required for explorative preclinical biomechanical investigations, as they can potentially account for the complex physics of the intervertebral disc environment, such as the fluid-solid interactions within the implant as well as the interaction between the implant itself and the surrounding intact biological structures, which involve the contact between nonlinear and nonhomogeneous multi-phasic materials. For that purpose different disc replacement configurations were evaluated on how they affect the response of a poroelastic finite element model of the intervertebral disc under complex physiological loads.

2) Vascular transport model

Using a poromechanical finite element (FE) model coupled to a transport model we studied the effect of mechanical and nutritional factors on the diffusion of two fundamental cell solutes, oxygen and lactate, strongly related with disc cell metabolism1. In our model crucial disc properties such as fluid content, osmotic pressure of the nuclear region, disc height, permeability, cell density, pH, were parameterized and their effect was studied on both the mechanical and solute transport response. Importantly, disc mechanical response to external compressive loads was simulated at the same time. External compressive loads affected oxygen and lactate contents within the disc. Sustained compression had its greatest influence on nutrient transport by decreasing diffusion distances diffusivity of solutes. We found that the more the disc was deformable, the larger was the effect. By comparing with in vivo literature data the model predicted similar oxygen and lactate patterns. A parametric study showed that the most important factors affecting the solutes' transport were: cell density, fluid content, disc height and nucleus osmotic pressure while other parameters had no effect. It is also important that a model should be able to account for the detrimental effect of acidic pH (due to lactate accumulation) which is the most relevant nutrient affecting cell viability.

Project Acronym and Number: Disc Regeneration—213904
Project Title: Novel biofunctional high porous polymer scaffolds and techniques controlling angiogenesis for the regeneration and repair of the degenerated intervertebral disc
Start and End Dates: 01/11/2008 till 31/10/2012
EU Contribution: 6.977.150€
Coordinator: LUIGI AMBROSIO, ambrosio@unina.it

Modelling

in DYNAMAG 233552

Subject of the modelling
Dynamics in magnetic nano-materials and devices

Models used
Ab-initio models for the exchange interaction, magnetic anisotropy and magnetization.
Micromagnetic models based upon the Landau-Lifshitz equation with ab initio parameters to calculate the spin wave spectra and dispersion in multilayer structures.
Models of relative dynamics of different sublattices in antiferromagnetic and ferrimagnetic materials
Models of spintronic and magnonic devices
Models of electromagnetic absorption and emission in magnetic nanomaterials

Simulation software and type of numerics used
NMAG
VASP and WIEN2k (ab-initio)
Finite difference micromagnetic packages, including parallel version of OOMMF and a code based on the Dynamical Guiding Centre approximation (GCA);
Finite element micromagnetic package Nmag
Dynamical matrix method (DMM) calculations
Micromagnetic data processing software SEMARGL and utilities for data transfer between Nmag and OOMMF (SEMARGL);
Plane wave method (PWM) calculations;
Monte Carlo calculations for spin lattice models
Parallel versions, in particular for multicore desktop PCs

Achievements of the model beyond experiments
The calculations pointed out samples that were until then simply not considered.
A novel magnonic logic architecture has been developed based on physics discovered by the models.
The, until then unexplained, origin of the response experimentally observed in optical pump-probe studies of magnetic multilayers with strong perpendicular magnetic anisotropy, has been revealed via calculations in the discrete lattice model.
Mechanisms behind unusually low magnetic domain wall depinning currents within spintronic devices have been revealed via full 3D finite element simulations.

Application
Spintronics and magnonics, including magnonic crystals, spintronic and magnonic devices interconnected with more conventional photonic, plasmonic, and electronic devices.

Relevant review articles:
S. - K. Kim, “Micromagnetic computer simulations of spin waves in nanometre-scale patterned magnetic elements”, J. Phys. D – Appl. Phys. 43, 264004 (2010).

Summary of project

Dynamag is a modelling project that focusses on magnonic crystals, a sub-field of a wider field of research called magnonics, and also deals with nanomagnetism and more specifically spin dynamics in magnetic nanomaterials and nanodevices. The ability to accurately predict fundamental and functional properties of fabricated magnetic nanostructures and complete devices by theoretical means is based on a thorough understanding of the relation between their chemical and physical fine structures and the desired useful magnetic functionalities.

Summary of the modelling

Competition between long and short range magnetic interactions leads to inherent complexity of phenomena observed in magnetic structures with nanoscale features, and hence to dramatic difficulties in their analytical treatment.
DYNAMAG has extended the mathematical formalism of numerical micromagnetic solvers beyond the classical Landau-Lifshitz equation by a rigorous account of spintronic and thermodynamic aspects of modelled phenomena occurring in multi-sub-lattice magnetic materials. DYNAMAG also developed new software applications to process and analyse large amounts of data produced by micromagnetic simulations, in particular those run using supercomputers.

(a) The finite element micromagnetic package Nmag (http://nmag.soton.ac.uk) has been extended to explicitly simulate relative dynamics of different sub-lattices in ferrimagnets and antiferromagnets and to facilitate inclusion of various spin transfer torque terms within models of magnonic devices interconnected with those of magneto-electronics (spintronics). This inclusion has provided deeper insights into the dynamical performance of magnetic sensors and recording heads.

(b) The dynamical matrix method (DMM) code has been further developed, in particular to facilitate the calculation of the Brillouin Light Scattering (BLS) cross-section from the DMM results. The complete 2D magnonic band structure (and the resulting magnonic dispersions) has been successfully reproduced and interpreted.[S. Tacchi, et al, Phys. Rev. Lett. 107, 127204 (2011)].

(c) A new dynamic simulation code based on the guiding centre approximation (GCA) has been developed, which can be interpreted as slow-variable micromagnetism.

(d) A micromagnetic code particularly for studying static magnetic configuration and time domain dynamics of magnetic vortices in arrays of magnetic discs has been developed.

(e) A new software tool called SEMARGL (http://www.magnonics.org/semargl/) has been developed to facilitate comprehensive analyses of large volumes of data produced by micromagnetic calculations. A new methodology has been developed to use the tool for calculating the scattering parameters of spin waves from magnetic non-uniformities, the magnetic susceptibility and permeability of magnonic metamaterials, as well as the magneto-optical signal measured in optical pump-probe experiments.

(f) A new software utility for Nmag that allows one to convert its output into the OVF format of OOMMF.

(g) The plane wave method (PWM) has been developed to calculate magnonic dispersion relations in samples that are currently in focus of experimental studies.

http://www.dynamag.eu/

Project Acronym and Number: DYNAMAG 233552
Project Title: Advanced Computational Studies of Dynamic Phenomena in Magnetic Nanomaterials
Start and End Dates: 01/06/2009 till 31/05/2012
EU Contribution: 899.936 €
Coordinator: Volodymyr Kruglyak, University of Exeter, UK, V.V.Kruglyak@exeter.ac.uk

Modelling

in FEMTOSPIN 3281043

Subject of the modelling

Heat-assisted or optically induced ultrafast reversal of magnetism

Models used

First principles electronic method:

Time-dependent spin density functional theory (TDSDFT) with spin scatteringeffects.

Atomistic models

Models using Heisenberg formalism including thermodynamics with improved dissipation and energy transfer mechanisms expressed by Langevin dynamics for non-zero temperatures.
Heat bath models (new development) directly simulating the behaviour of the excited conduction electrons coupled quantum mechanically to atomic spins. The atomistic parameters calculated are the temperature dependence of magnetisation and of a longitudinal and transverse susceptibility and are input to the macrospin model.
(10^8 spins, 2-D structures of up to 1000nm, and the timescale is now up to ns)

Mesoscale models

Micromagnetic (macrospin) model including quantum effects based on the generalised Landau-Lifshitz-Bloch equation for ferrimagnets, antiferromagnets and magnetic semiconductors

Simulation software and type of numerics used

Budapest code based on the kkr code using spin-cluster expansion technique to calculate ab-initio parameters (spin, exchange integrals, anisotropy).
Uppsala code for TDDFT calculations to understand the origin of the optomagnetic field.
VAMPIRE (Visual Atomistic Massively Parallel Integrator Engine) for atomistic calculations of dynamic response to ultrafast laser pulses.
York code for heat bath models, used to understand the underlying processes of energy transfer between the excited conduction electrons and the spins.
Madrid/Konstanz code for micromagnetics with finite-difference discretisation for large-scale calculations for comparison with experimental data, especially imaging.
Transfer of data between models;
Ab-initio information (spin, exchange integrals, anisotropy) used to parametrise atomistic and heat bath model calculations.
Atomistic models used to calculate information (temperature dependence of magnetisation, anisotropy and longitudinal and transverse susceptibilities) for use by mesoscopic models

Achievements of the model beyond experiments

Prediction efficiency of ultrafast spin dynamics in multiferroics excited by THz laser pulses
Prediction of the smallest stable domain structure in magnetic thin films
Prediction of the time and spatial scales of magnetic pattern formation
Identification of optimal materials for ultrafast optically induced magnetic switching

Application

Magnetic recording with increased speed of logic and data storage devices with increased storage density, Novel ICT-devices based on spin manipulation

Relevant review articles

I Radu et al, Ultrafast magnetism as seen by x-rays, Proc. SPIE 8260, 82601M (2012); http://dx.doi.org/10.1117/12.907433

Summary of project

The project addresses spin dynamics for magnetic information storage technology, which is based on nanostructured magnetic materials, and for spin electronics in which the manipulation of the spin forms the basis of the device operation. Magnetic spins can be manipulated on the femtosecond timescale, while the actual switching by precessional motion lasts hundreds of picoseconds. The project investigates the physics of these multi-scale processes.

Summary of the modelling

The standard formalism used for materials and device simulations (micromagnetics) is a continuum formalism dealing with the spin precession timescale of 10ps upward. However, optical spin manipulation and magnetisation processes are intrinsically much faster than that of precessional switching e.g. complete demagnetisation happens on the timescale of hundreds of fs. Thus multi-scale models are required dealing with the timescales associated with exchange, spin-orbit coupling and spin-flip scattering.
The project will investigate processes at the light-spin interaction level, electronic structure level, atomistic level and mesoscale level.
The fundamental interactions between spin, conduction electrons and the laser light (excitation and demagnetization processes) that occur on very short time scales (atto- to femto-seconds) will be described and the beyond- linear-response real-time formulations shall be combined with ab-initio code on the basis of the time-dependent spin-density functional theory (TSDFT) to compute ultrafast magneto-optical response.
The inverse Faraday effect is at the origin of the laser-induced “optomagnetic” field and this mechanism is further investigated so that it can be implemented in the atomistic spin Hamiltonians used in atomic simulations.
A model of non-equilibrium spin-scattering (energy and spin transfer) channels will be built that can predict ultrafast demagnetization. The aim is to develop a suitably parameterized form of demagnetization caused through hot electron transport that can be used and incorporated in the spin Hamiltonians used for atomic simulations. The temperature dependent ab-initio parameters of spin Hamiltonians can be used in the atomistic spin-dynamics simulations. The first-principle electronic structure will be mapped to a multiband Hubbard model, with realistic tight-binding and interaction parameters. Within the framework of the multiband Hubbard model, the effects of exchange interactions being different from those in equilibrium (non-adiabatic effects) will be studied.
The project will introduce the above mentioned physics into the atomistic lengthscale heat bath models which rest on fixed spin length and fixed model parameters. They will develop equations of motion beyond current Langevin dynamics to arrive at a better treatment of the coupling of the spin system to electronic and phononic degrees of freedom and hence a better modelling of the dissipation channels. Also a more realistic model for the energy transfer on the fs timescale will be included. The coupling between the atomic spins and the heat bath will be based on the ab-initio models developed. To identify optimal materials for ultrafast optically induced magnetic switching the relevance of the specific spin ordering in ferro-, ferri-, antiferro-magnetic and magnetic semiconductors will be studied.
The project will include quantum effects in macrospin models of ferrimagnetic and antiferromagnetic materials. These macrospin models are based on the micromagnetic approach with finite-differences discretization and use the input of the electronic structure and atomic models. The codes will be used for (granular and polycrystalline) materials design exercises for heat assisted magnetic recording. The atomistic and multiscale spin models, developed within ULTRAMAGNETRON and FEMTOSPIN are providing important insight into the physics of Heat Assisted Magnetic Recording (HAMR), and the testing and validation carried out within those projects are leading to the point at which the computer models are ready to become predictive design tools.

http://femtospin.eu/

Project Acronym and Number: FEMTOSPIN NMP3281043
Project Title: Multiscale modelling of femtosecond spin dynamics
Start and End Dates: 1/6/2012 till 30/6/2015
EU Contribution: 3.999.500 €
Coordinator: Roy Chantrell, University of York, UK, roy.chantrell@york.ac.uk

Modelling

in FREECATS 280658

Subject of the modelling

Catalysis reactions and processes in foam structures

Models used

Multi-scale model for mass transfer, heat transfer, kinetics and hydrodynamics in foam structures

Simulation software and type of numerics used

MODELICA, MATLAB custom systems of partial differential equations with commercial PDE solvers; ANSYS CFD based code with custom reaction code written in C++

Achievements of the model beyond experiments

Heat transfer modelling guides the design of the foam materials and predicts the deposition of carbons during operation, (a phenomenon critical in oxidative dehydrogenation) and so reduce costs of trial and error developments.

Multi-scale modelling of reaction, surface-fluid interactions, heat transfer and hydrodynamics allow to predict from first principles the behaviour of the overall reactor system and to screen a large space of operating conditions prior to experimentation. This leads to better understanding of physical phenomena involved and dynamics of processes within the system, thus reducing the number of experimental trials required.

Application

Catalysts, reactor design

Relevant review articles

Kambiz Chizari, et al Nitrogen-Doped Carbon Nanotubes as a Highly Active Metal-Free Catalyst for Selective Oxidation: ChemSusChem (2012) DOI: 10.1002/cssc.201100276

Summary of the project

This project is addressing catalysis for the sustainable production of chemicals and commodities. The FREECATS project deals with the development of new metal-free catalysts, either in the form of bulk nanomaterials or in hierarchically organized structures both capable to replace traditional noble metal-based catalysts in catalytic transformations of strategic importance. Metal-based catalytic processes are considered in the light of new tailored metal-free catalytic architectures designed and fabricated starting from appropriate nanoscale building blocks.

Summary of the modelling

The models to be developed will address the chemical reactions, heat and mass transfer, and hydrodynamics with the foam structure as a parameter.

Based on the data on catalysts characterisation and kinetic measurements an analytical mechanistic reaction kinetic model will be developed and validated against the available data. The code solving the equation will be developed in MODELICA, which is an open-code modelling environment. The code will later be transferred (as custom-routines coded in C++) into commercial software (ANSYS). The model will be used to detail surface reactions and adsorption processes of the new catalysts.

A micro-model of heat conduction through a foam material based on the solid mechanics package within ANSYS and using finite elements methods will be applied. For this the actual structure of the foam, obtained through electron tomography, and geometrical models of the foam structure, will be used.

Two process models will be applied:

In the first approach, the above described kinetic MODELICA model will be coupled to MODELICA gas-solid, gas-liquid and gas-liquid-solid mass transfer models, heat transfer and hydrodynamics. These continuum models will ignore inertia effects. The MODELICA code will be used for process optimisation. The model will explore a wide range of operating conditions. The key part of the model will be the part of the code relating foam structure to heat and mass transfer characteristics. This will be a semi-empirical model, as ab-initio model is unnecessarily complex for the desired outcome.
In another approach to describe the total process a CFD code describing the foam geometry at a coarser level to represent the continuous fluid domain will be run. Information from the MODELICA kinetics model will be fed in via boundary conditions detailing surface reactions and adsorption processes. The CFD model will take into account complex physical processes, resolving heat, mass and momentum transport in boundary layers and accounting for inertia. The purpose will be to resolve macroscopic heat, mass, momentum transport everywhere in the foam.

www.freecats.eu

Project Acronym and Number: FREECATS 280658
Project Title: Doped carbon nanostructures as metal-free catalysts
Start and End Dates: 01/04/2012 till 31/03/2015
EU Contribution: 3.955.619 €
Coordinator: Professor Magnus Rønning, NTNU, magnus.ronning@chemeng.ntnu.no

Modelling

in GOFAST 280555

Subject of the modelling

Optical control by intense ultra-fast laser pulses of metallic phases in the prototypical Mott insulator V2O3 and of the superconductive phase in the high-temperature superconductor family BSCCO.

Models used

Models for correlated systems: Multi-orbital lattice models of the Hubbard type
Time-dependent Dynamic Mean Field Theory (DMFT) for out-of-equilibrium evolution
Time-dependent Gutzwiller variational approach

Simulation software and type of numerics used

Continuous-Time Quantum Monte Carlo (CTQMC) and Exact Diagonalization (ED) for solving the DMFT model
Iterated Perturbation Theory (IPT)
Multi-dimensional optimization for the time-dependent Gutzwiller model
Solving a set of non-linear Schroedinger equations for evolution of the wavefunction

Achievements of the model beyond experiments

The model identified optimal correlated materials (composition, size, direction of the laser pulse versus surfaces, etc) and excitation pathways (photon energy, intensity, polarization and temporal profile) for the production of controllable and reversible photo-induced transitions between distinct phases, e.g. metallic and insulating, or normal and superconducting.

Application

Switching devices based on the optical switching between phases with very different conducting properties.

Relevant review articles:

Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, Antoine Georges, et al Mod. Phys. 68, 13 (1996)
The Out-of-Equilibrium Time-Dependent Gutzwiller Approximation, M. Fabrizio, arXiv: 1204:2175 (2012).
Non-equilibrium dynamics of the driven Hubbard model, A. Amaricci, et al, arXiv:1106:3483 (2011).
Time-Dependent Mean Field Theory for Quench Dynamics in Correlated Electron Systems, Marco Schiró and Michele Fabrizio, Phys. Rev. Lett. 105, 076401 (2010)

Summary of project

The aim of this research project is to develop femtoscale-modelling schemes to study electronic, optical and structural properties of correlated materials driven out of equilibrium. The possibility to optically switch on and off the metallic phase in a model Mott insulator (vanadium sesquioxide) and the superconducting phase in model high-temperature superconductors (cuprates) will be investigated and tested. The photo-excited phases are investigated experimentally by different time-resolved spectroscopic tools, like reflectivity or photoemission.

Summary of the modelling

GOFAST will extend techniques for correlated systems, i.e. Dynamical Mean Field Theory (DMFT) and the Gutzwiller variational approach, to model the temporal evolution after high-energy excitations are impulsively photo-injected by ultrafast laser pulses. DMFT is a quite accurate technique, although numerically very demanding. The Gutzwiller approach is less rigorous but very flexible, relatively easy to implement and to push towards long simulation times. An important step to be undertaken is finding the minimal models able to provide a reliable description of the materials under investigation, where minimal means the minimum amount of complexity.
These models aim at describing the properties of a subset of electrons that participate to conduction and where correlation effects are predominant. In transition metal oxides these electrons are commonly those that reside on the partially filled d-shell of the transition metal ions (as opposed to light elements where the p-shell electrons control the properties). If one assumes that all the other occupied shells, both of the transition metal ions and of the oxygen's, just provide an effective potential for the d-electrons that adds to the ionic one, then the effective Hamiltonian projected onto the d-like Wannier orbitals has generally the form of a tight-binding model of ~~the~~ interacting conduction electrons. Besides a long-range part, the electron-electron interaction comprises also a short-range contribution that includes a charge-repulsion, so-called Hubbard U, and an exchange splitting responsible for the Hund's rules. In vanadium sesquioxide, each V donates three electrons to the oxygen's; hence there remain two electrons to accommodate into the t2g–orbitals that derive from the original five d-orbitals split by a cubic field. In this situation, Hund's rules play an important role. In addition, a trigonal field further splits the t2g–orbitals into a doublet and a singlet, e_{ng} and a_{1g}, respectively, and the phonon mode that controls such a splitting is known to play an important role in all physical properties. In BSSCO cuprates only one among the crystal field split d-orbitals is involved in the physics, which is a simplification with respect to V2O3. However, antiferromagnetic fluctuations are known to play an important role in these materials, hence these have to be taken into account either explicitly or via an effective bosonic mode. When needed, realistic Hamiltonian parameters will be extracted from ab-initio LDA-DFT calculations through the Quantum Espresso Density Functional package
The other crucial task is to extend DMFT and the Gutzwiller variation approach for studying out-of-equilibrium conditions provoked by an intense ultrafast laser pulse. The simplest models will be studied both at equilibrium and out-of-equilibrium and the results compared with experiments. If the agreement is not satisfactory, additional ingredients suggested by the experiments will be included in the models, which will be once again analysed at equilibrium and out of it. The procedure will continue till the modeling will compare well with experiments.

Project Acronym and Number: GOFAST 280555
Project Title: Governing ultrafast the conductivity of correlated materials
Start and End Dates: 01/04/2012 till 31/03/2015
EU Contribution: 1.673.200 €
Coordinator: Michele Fabrizio, University of Trieste, Italy, fabrizio@sissa.it

Modelling

in HIPERSOL 228513

Subject of the modelling
Resistance and recombination of charges at interfaces in solar cells

Models used
Electronic
First principle (DFT) method to construct inter-atomic potentials (up to 2000 atoms)
Semi-empirical electronic calculations calculate electronic structure of large structures with up to millions of non-equivalent atoms and calculate the lifetime of charge carriers
Atomistic
Classical Molecular Dynamics using DFT-constructed inter-atomic potentials
Statistical temperature accelerated molecular dynamics and kinetic Monte-Carlo to calculate diffusivities of charge carriers, band structure calculations for up to 10000 atoms
Continuum, Thermodynamics
Phase field modeling of dissolution of Ag particles and transport of Ag through the amorphous glass layer to the bulk Si

Simulation software and type of numerics used
VASP and extensions for DFT based on matrix diagonalisation procedures for plane wave based Hamiltonians
DL-POLY used for empirical molecular dynamics based on velocity and leapfrog Verlet integration schemes
LAMMPS used for empirical molecular dynamics and energy minimization applying special-decomposition techniques
FactSage used for estimation of Gibbs free energies
COMSOL for transport model (conductivity) of current flow through the interface region and phase field model of the firing process. Based on solution of large sparce systems

Achievements of the model beyond experiments
The methods can predict contacting and recombination properties of nanostructured materials and complicated interfaces.
The model gave fundamental insight into nitrogen diffusion in silicon, into the nature of different recombination traps, into dissolution and transport of Ag during the firing process, and insight in how the current flows through the contacting region. Based on this optimal Ag crystallites geometries were gained.

Application
Optimisation of contacting and passivation schemes for solar cells

Relevant review articles:
K.T. Butler, et al. Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. Phys. Rev. B 83, 235307, 2011
Keith T. Butler, et al. Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. J. Appl. Phys. 110, 124905, 2011
G. Kresse et al. Optical and electronic properties of Si3N4 and α-SiO2. Phys. rev. B 85, 45205, 2012
M. Marsman, G. Jordan, L.-E. Hintzsche, Y.-S. Kim, and G. Kresse. Gaussian charge-transfer charge distributions for non-self-consistent electronic structure calculations. Phys. rev. B 85, 115122, 2012

Summary of project
The HIPERSOL project will address the improvement of solar cells (beyond bulk calculations of band gaps) via modelling reflecting the complexity of the real surfaces and want to include impurities and defects which determine the performance in practice. Included will be the effects of recombination (at the interface between base (passivation layer) and emitter (semiconductor) and resistive losses (at this interface and at the metal contact-emittor interface) as they are the major loss mechanisms for the light generated carriers (electrons and holes).

Summary of the modelling
HIPERSOL is to develop an integrated multi-scale modelling environment that is applicable to properties of real materials on length scales not accessible by ab initio modelling; and to use this environment to accurately describe and predict important parameters and properties of interfaces of contacting and passivation layers with silicon. HIPERSOL targeted to do fully self-consistent DFT band structure calculations for systems containing up to 10.000 atoms, as the typical extension of such interfaces easily stretches to hundreds of nanometres. This is done integrating ab initio calculations with empirical atomistic modelling and finite-element methods.

First the construction of inter-atomic potentials was derived from first principles calculations (0.1-1 nm). These inter-atomic potentials were used in empirical molecular dynamics (EMD) performed on the most relevant and interesting interfacial regions of the contacting and passivation interfaces, accounting for strain and for misfit dislocations. The EMD simulations provided input for DFT calculations of the contacting interface. The Si/Ag and Si/Ni interfaces have been generated using EMD and based upon derived inter-atomic potentials. These structures have been used to calculate Schottky barriers from DFT. The passivation (Si/SiNx) interface has also been modelled with inter-atomic potentials developed. These simulations were used to investigate the influence of N content and gradients on the trap density at the interface.

To apply DFT at a much larger scale than done until now, semi-empirical pseudo-potentials (SEPP) (10-100nm) were created based on first-principles calculations on a smaller scale (density functional theory, hybrid functionals and the GW approximation). These screened potentials can be used within the framework of DFT to calculate the accurate electronic structure of large structures with up to millions of non-equivalent atoms and calculate life times of charge carriers
The atomic coordinates at quasi-equilibrium were transferred to, and formed the basis for the rest of the first principle modelling in this project. Diffusivities and surface energies were also extracted as input to the modelling of the metallisation process. The extraction of diffusivities required including methods from temperature-accelerated molecular dynamics and kinetic Monte Carlo simulations.

In a following stage, results from EMD and first principles calculations (such diffusion parameters and surface energies) were used as input to finite element method calculations, reaching the size and time scales of real devices.

To support the above, numerical techniques were developed for accurate calculation of electronic band structures in sub-systems large enough to include macroscopically relevant features. This involved the integration of realistic band structures and first principles wave functions in the envelope function approach, which were used to calculate life times of excited charge carriers.

Calculations have been performed on novel stacked Si/SiNx structures and new model paste compositions for metallisation under different firing conditions to improve contacting and passivation schemes. The applicability of new pastes was assessed to industrial production. The transport of Ag from the finger through the glass layer to the bulk silicon was modelled with a phase-field model, based on Gibbs free energies obtained from FactSage (using a database developed for solar grade silicon) and diffusivities obtained from first principles molecular dynamics.

www.sintef.no/Projectweb/HiperSol

Project Acronym and Number: HIPERSOL 228513
Project Title: Modelling of interfaces for high performance solar cell materials
Start and End Dates: 01/12/2009 till 31/11/2012
EU Contribution: 3.399.990 €
Coordinator: Jesper Friis, SINTEF, Norway, jesper.friis@sintef.no

Modelling

in HIVOCOMP 246389

Subject of the modelling

Composites consisting of a matrix and textile fibrous reinforcement (woven carbon fabric).
Self-reinforced composites consisting of a matrix and the reinforcement of the same chemical nature (polypropylene or polyamide).

Models used

Microscale model for Newtonian fluid flow in porous medium (fibres inside the yarns)
Mesoscale (unit cell of the textile reinforcement) model for uncompressible fluid (resin) flow through the textile reinforcement (Navier-Stokes/Stokes and Brinkmann equations) resulting in calculation of the homogenized permeability.
Micro-mechanics models (elasticity and plasticity and fracture) to calculate the deformation resistance (compression, shear, tension, bending) of dry preform and stiffness and strength of the impregnated composite.
The results of the micromechanics modeling are used in macro-level models for simulation of forming and impregnation and finally the structural behavior of the part.
Geometrical description of the reinforcement is the starting point of all the models.

Simulation software and type of numerics used

PAM-RTM a Darcy solver to simulate flow of Newtonian liquid through a porous medium (impregnation of a composite part)
FlowTex for micro scale Stokes, Navier-Stokes and Brinkmann flow
WiseTex a micromechanics software to compute the internal structure and deformability of textiles;
PAM-family of ESI for macroscale forming.
All flow models use finite difference and mechanical models use FE technology

Achievements of the model beyond experiments

Prediction of structural properties to avoid unfeasible or expensive experimental tests.
The models also enabled screening of possible choices for the resins. The flow modeling shortened part of the design by predicting permeability and impregnation time of the different resins.
The model predicted structural behavior in function of the above properties and damage initiation by calculating the threshold and damage development parameters in the composite during different loading types

Application

Composite parts for the transport industry

Summary of the project

HIVOCOMP focuses on improving two materials systems for high performance carbon fibre reinforced parts and their production. The materials systems are: 1) advanced polyurethane (PU) thermoset matrix materials (resin) reinforced with textile (carbon) fibres and 2) composites consisting of self-reinforced thermoplastic polypropylene and polyamide composites, incorporating carbon fibre reinforcements.

Summary of the modelling

HIVOCOMP models the flow of the novel low-viscosity resin impregnating the network of textile reinforcements at meso and macro scale which is performed with an existing finite difference model for Newtonian flows in porous media and Stokes, Navier-Stokes and Brinkmann flow in the network of fibrous reinforcements.

The modelling starts with a geometrical description of the textile. Micromechanics models for mechanical deformation and shrinkage will lead to the description of resistance of the hybrid (carbon/self reinforced PP or PA) preform to deformation and shrinkage during thermoforming. The models will produce material constitutive equations to be used in the macro-modelling of forming.

Novel, predictive micro-mechanics models of elasticity are used to model damage and toughness of the materials following two routes:

1. Micro-level mechanics/elasticity model of textile reinforced PU composite and self-reinforced PP/PA. To account for the specific adhesion behaviour of carbon fibres in PP/PA, special finite elements will be introduced in the calculations. Novel theory of distributed damage, based on Ladeveze-type damage parameters and Puck-type damage initiation criterion is implemented in the model. An alternative predictive approach suitable to crack initiation and growth and based on the existing nonlocal damage EWK (ESI-Wilkins-Kamoulakos) model will also be used and coupled to the MultiModel Coupling capability of PAM-codes to achieve immediately simulation capabilities of industrial dimension.
2. Fast simulation using method of inclusions (Eschelby and Mori-Tanaka) of strength and damage-induced deterioration of the stiffness of composite including strength analysis of the equivalent inclusions and degradation of the stiffness of the inclusions. The method of inclusions is based on Eshelby's transformation concepts, and uses a short fibre analogy to describe the mechanical behaviour of curved yarn segments, combined with a Mori-Tanaka or self-consistent scheme to account for interaction effects. The geometrical input from WiseTex consists of the yarn mid-line representations and cross-sectional dimensions. Yarns are split up into segments and replaced by a short fibre equivalent using the yarn orientation and the local curvature. The output of the model is full stiffness matrix of the homogenised unit cell. In the elasticity model the orientation and length distribution of the fibres are used to generate instances of the random placement of the inclusions. Monte-Carlo scheme is then used to calculate homogenised stiffness matrix

Deterioration of stiffness of the composite with increased loading is calculated in the form of non-linear stress-strain diagrams. This approach lacks the thoroughness of meso-FEA, but will allow integration into the macro-level structural analysis of the composite part.

Finally the developed micro-meso level models are implemented in macro simulation tools PAM- family (ESI).

http://hivocomp.eu/

Project Acronym and Number: HIVOCOMP 246389
Project Title: Advanced materials enabling HIgh-Volume road transport applications of lightweight structural COMPosite parts
Start and End Dates: 01/10/2010 30/09/2014
EU Contribution : 4.775.278€
Coordinator: Ignaas Verpoest, KU Leuven, BE, (+32 16 321306) ignaas.verpoest@mtm.kuleuven.be

Modelling

in HYMEC 263073

Subject of the modelling

Organic semiconductors

Models used

drift-diffusion models, TDDFT, Hubbard model, percolation model

Simulation Software and type of numerics used

TIBERCAD (commercial, but developed in part by partner of HYMEC). Monte Carlo algorithm to solve percolation model

Achievements of the model beyond experiments

The electric field distribution of charged metal nanoparticles in organic matrices can be predicted, which allows identifying the switching mechanisms of memory cells. This, in turn, allows optimizing the morphology of devices.

Application

Photonics and electronics

Summary of project

The goal of the project is to investigate all relevant properties of systems comprising inorganic metal nanoparticles embedded in matrices of conjugated organic materials (organic semiconductors) and demonstrate the potential of such material hybrids as non-volatile memory elements (NVME) that can be addressed electrically and optically. This will allow interconnection of future hybrid electronic and photonic circuitry. Moreover, we target implementing cost-efficient production routes, such as printing, as well as exploring the ultimate miniaturization of such memory elements by novel sublimation- and imprinting-based nanostructuring processes.

Summary of the modelling

The theoretical work consist in developing computational tools for the structure-property-function relationships for NVMEs based on metal NPs embedded in organic matrices, with the view of expanding the functionality of NV-MEs towards optical addressing capability and allow cost-efficient fabrication methods (printing and nanostructure formation).
A macroscopic model will be used to simulate electrical characteristics of steady-state transport in the two different conduction states. The effect of optical addressing the device to induce charging and de-charging of the metal NPs in the macroscopic device is included in the modelling tool.
Improving an existing a multiscale code called TiberCAD we will study recombination mechanisms.
A drift-diffusion model has been already implemented with several submodels for recombination and charge mobility (in particular a field dependent mobility). It includes also a module to include a fixed charge background and is currently going on the development of a module to include trapping and de-trapping models, both for energy localized traps or for more extended band-tails (like in amorphous materials). This computational tool will be used to model the device in steady state conduction when it is in high conductivity state or low conductivity state, respectively. Experiments will provide information on adequate rate equations for trapping mechanisms and charge mobility. Experimental results on the electrode/organic matrix interface energetics will be used to model the boundary conditions as Schottky-barriers at the contacts.
A percolation model can be easily grasped using a random walk (RW) over a network of nodes, every of which, representing a metal NP and so a possible site for charges, connected to a certain number of other nodes. The problem is solved using a Monte Carlo method and solving a Pauli Master Equation.
The main parameters for this model are related to the jump rate and the coordination numbers (substantially related to the density of NPs) and can be phenomenologically with well-known methods of quantum field theory and the support of experimental measurements.
The most demanding part of the theoretical work is the inclusion of exciton creation, transport and recombination (including charging and de-charging of metal NPs) to grasp optical addressing in the drift-diffusion model and the RW model.
In that case the Hamiltonian of the system is described by a Hubbard model but with a strong correlation term between particles. We will investigate this by density matrix renormalization group (DMRG) for the ground state properties and by time-dependent mean-field theory (TDMFT) for transport properties.
A software package is developed to model transport through NV-MEs including the main physical processes which affect conduction, such as charge effects, trap and de-trapping processes.
When the simulation tool is well tested and established as being reliable, it will be used as a support for the further engineering of devices, and it will be instrumental for the development of array and integration efforts in order to find the best selections of materials and device architectures.

http://hymec2.physik.hu-berlin.de

Project Acronym and Number: HYMEC 263073
Project Title: Hybrid organic/inorganic memory elements for integration of electronic and photonic circuitry
Start and End Dates: 1 October 2011 till 31 September 2014
EU Contribution: 3.132.475 €
Coordinator: Norbert Koch, Humboldt-Universität zu Berlin, Institut f. Physik, Germany;
norbert.koch@physik.hu-berlin.de

Modelling

in HYPOMAP 233482

Subject of the modelling

Hydrogen storage materials (physisorption and chemisorption), ad- and desorption processes, and proton exchange membranes.

Models used

Electronic structure models for hydrogen adsorption including
Density-Functional Theory (DFT) and Quantum Monte Carlo to solve the many body problem.
Ab initio calculations (MP2, CCSD(T))
Molecular dynamics

Simulation software and type of numerics used

Gaussian09, VASP, deMon2k, GPAW, TurboMOLE
Various Order-N techniques are used, including (i) diagonalization methods, (ii) Fast Fourier Transform, (iii) Matrix-matrix linear algebra operations, (iv) solvers for systems of linear equations.
Monte Carlo simulations using self-developed codes (i.e. QLDFT)

Achievements of the model beyond experiments

Computational modelling, in particular on the electron or atomistic scale, allows the investigation of processes beyond the experimental scale. People often speak of the “computer microscope” that allows to monitor the motion of a single atom. It also provides understanding of an individual vibrational mode, or of the contributions of material fragments to an individual property. In this project modeling provide insight in the adsorption energy of hydrogen as function of the composition of the individual building blocks of a molecular framework. With this data it is possible to improve the performance of the target materials.

Application

Hydrogen storage and fuel cells

Relevant review articles

R. B. Getman, Y. S. Bae, C. E. Wilmer, R. Q. Snurr, Chem. Rev. 112 (2012) 703-723, DOI: 10.1021/cr200217c.
S. S. Han, J. L. Mendoza-Cortes, W. A. Goddard III, Chem. Soc. Rev. 38 (2009) 1460-1476, DOI: 10.1039/b802430h.
S. A. Shevlin, Z. X. Guo, Chem. Soc. Rev. 38 (2009) 211-225, DOI: 10.1039/b815553b.

Summary of the project

Effective hydrogen storage and fuel cell systems are required for the implementation of a hydrogen economy. HYPOMAP uses computational approaches to predict hydrogen adsorption and proton transfer in new candidate materials for technological application.

Summary of the modelling

For hydrogen storage by physisorption, the weak interaction between the H2 molecules and the host structures need to be modelled in order to understand the thermodynamics of the system. For chemisorption, the critical steps are the loading and unloading, so the mechanism of catalysts on the storage systems needs to be modelled. For fuel cells, the proton conductance in the proton exchange membranes needs to be studied. In all cases, dependence on temperature and pressure are to be included.

All three properties are described by the Schrödinger equation, but approximated in different ways. For physisorption, as Kohn-Sham equations of a bosonic system of hydrogen molecules, for chemisorption as Kohn-Sham equations for electrons, and transition state theory is applied afterwards, while Born-Oppenheimer techniques in conjunction with transition state theory and molecular dynamics is used for the proton exchange membranes.

QLDFT (Quantum Liquid Density Functional Theory) was developed because there was no adequate modelling method for the adsorption calculations on the market that included the quantum effects of light-weight hydrogen. This was a considerable development effort, as (i) a physical method needed to be developed, implemented and validated; and (ii) a series of numerical techniques, treating very large sparse matrices (dimension of ~100,000) efficiently had to be implemented. The Moreover, we implemented an efficient technique to account for London Dispersion (a weak interaction governing the interaction of hydrogen with host materials) within DFT and implemented it into deMon2k.

https://www.jacobs-university.de/ses/theine/projects/HYPOMAP

Project Acronym and Number HYPOMAP 233482
Project Title: New materials for hydrogen powered mobile applications
Start and End Dates: 01/06/2009 till 30/05/2012
EU Contribution: 899.958 €
Coordinator: Thomas Heine, Jacobs University, DE, t.heine@jacobs-university.de

Modelling

in IMS & CPS

Subject of the modelling
Textile carbon fibre/epoxy composites reinforced with carbon nanotubes (CNTs), damage resistance, electrical conductivity and lightning strike protection

Models used
Microscale damage initiation model in textile fiber/reinforced composites
Conductivity model for polymer/CNT composites
Electrical, statistical, thermodynamic, structure based, electron tunneling percolation models

Simulation software and type of numerics used
WiseTex, TexComp for the calculation of stress and strain fields numerically in the representative volume using geometrical modeller WiseTex and commercial FE packages (such as ANSYS and ABAQUS).
Random Microstructure Generation (RMG) algorithm e.g. for buckling of the I beam with classic eigenvalue analysis.

Achievements of the model beyond experiments
The “electrical conductivity” model predicts the electrical percolation and conductivity of CNT/polymer composites close to the experimental observations. The achievements beyond experiments include the positive effect of agglomeration and the transverse conductivity of the CNT/polymer composite with the CNTs only sprayed on the surface. In fact, nobody believed that there will be conductivity in the transverse direction when the CNTs are sprayed on the surface alone. In addition, this model correctly predicted that the addition of compatibilizers and copolymers has a significant effect on electrical percolation threshold and conductivity. These characteristics are experimentally proved and this is the only model which can predict this behaviour.
The toughness model will predict the effect of carbon nanotubes and their agglomerates on re-distribution of stresses and strains inside the composite and the threshold strain for the onset of damage on the micro-scale.
The model utilized for validation elements can predict the initial failure of the T junctions and of the I beams for the different used materials (with and without CNT). This will help to design the test jigs to be used in the project.

Application
Textile reinforced composites, transport, aviation, railway

Relevant review articles
Verpoest I and Lomov SV, Virtual textile composites software WiseTex: Integration with micro-mechanical, permeability and structural analysis, Composites Science and Technology 65 (2005) 2563–2574.
Lomov, S.V., D.S. Ivanov, I. Verpoest, M. Zako, T. Kurashiki, H. Nakai and S. Hirosawa Meso-FE modelling of textile composites: Road map, data flow and algorithms. Composites Science and Technology, 67, 2007, 1870-1891
Weibang Lu, Tsu-Wei Chou, and Erik T. Thostenson. A three-dimensional model of electrical percolation thresholds in carbon nanotube-based composites. Applied Physics Letters, 96(22):223106, 2010.
Andriy V Kyrylyuk, Marie Claire Hermant, Tanja Schilling, Bert Klumperman, Cor E Koning, and Paul van der Schoot. Controlling electrical percolation in multicomponent carbon nanotube dispersions. Nature nanotechnology , 6(6):364 – 9, January 2011.

Summary of the project
IMS&CPS intends to gather innovations linked to carbon nanotubes based innovative materials and innovative composite processings for transport applications (aeronautics and railway applications).

Summary of the modelling
In order to achieve higher mechanical properties and higher electrical conductivities in multi-scale carbon fiber/epoxy composites, an important part of the IMS&CPS project is dedicated to the development of modeling methodologies and predictive tools. The goal of these tools is to help understand how to maximize the benefit of carbon nanotubes in the structural composites for the improvement of such properties as damage resistance, electrical conductivity and lightning strike protection. The success of this modelling lies in the geometric modeling of the CNTs, polymer chains and their interactions because the geometrical distribution of the CNTs in the representative volume has a significant impact on the electrical conductivity and the percolation threshold.

Representation of the sample
The software package WiseTex implements a generalised description of internal structure of textile reinforcements on the unit cell level, integrated with mechanical models of the relaxed and deformed state of fabrics. TexComp uses the geometrical input from WiseTex, which consists of the yarn mid-line representations and cross-sectional dimensions. Yarns are then split up into segments and replaced by a short fibre equivalent using the yarn orientation and the local curvature. The output of the model is full stiffness matrix of the homogenised unit cell. The representation is further refined using the random microstructure generation (RMG) algorithm to simulate a fiber distribution in the representative volume element. In the framework of the IMS&CPS it is proven this algorithm generates microstructures that are statistically equivalent to real microstructures (from the point of view of geometrical characteristics and mechanical performance). The modified version of this model is currently in the development, which goal is to simulate fibers and nanotubes in a single model without transferring parameters from simulations on one scale to another. This is mainly explained by numerical challenges that come from modeling objects that differ in dimensions by 1000 times (microscopic fibers and nanoscopic tubes).

Physics and chemistry
The above internal geometry and stiffness prediction is a necessary input for physics and chemistry modelling.
The damage initiation model is developed on the micro-scale. This model predicts transverse damage initiation in unidirectional fiber/polymer composites with and without carbon nanotubes.
The conductivity model for polymer/CNT composites predicts electrical percolation thresholds and electrical conductivity of polymers reinforced with CNTs. It can be applied to different kinds of CNT/polymer nano-composites. The model accounts for the two types of charge transport mechanisms with and without chemical bonding between CNTs and the polymer. In the first case creation of ions and charge transport through CNTs and polymer chain networks play a role, while in the second case charge transport through the physical contact between CNTs, through the electron tunneling between CNTs , through the electron tunneling between polymer chains and through the electron tunneling between CNTs and polymer chains are important.
To model the transport, thermodynamic percolation models are used, which emphasize the importance of the interfacial interactions at the boundary between the individual filler particles and the polymeric host for the network formation. As a consequence, these models interpret the percolation phenomena as a phase separation process.
Electron tunnelling is described with quantum mechanical percolation models which assume the charge transport between carbon nanotubes are partly through physical contacts and partly through electron tunneling between carbon nanotubes.

Representation of the sample
Different calculations are done to find a representation of where the fibers are after the physics and chemistry have evolved. Statistical calculations of random placement during dispersion and further agglomeration of carbon nanotubes give networks of physically connected paths. This is further refined in geometrical calculations to obtain a representation of the fibres in different dry premixed and subsequently sintered mixtures of conductive and insulating powders. Structure oriented models based on the parameters that have to be determined from the micro level structure of the mixture after final processing step. A detailed substitution of the real material structure by a theoretical model structure is needed for the determination of such parameters.

www.imscps.eu
Project Acronym and Number: IMS&CPS 246243
Project Title: Innovative material synergies and composite processing strategies
Start and End Dates: 01/10/2010 till 31/09/2013
EU Contribution : 4.925.711 €
Coordinator: André Bertin, COEXPAIR S.A., BE coordimscps@coexpair.com

Modelling

in INNOVASOL 227057

Subject of the modelling
Excitonic solar cell materials (QuantumDots, Transparant Conductive Oxides and solid electrolyte)

Models used
Ab initio Hartree-Fock and Density Functional Theory, SCF calculations of structures, electronic distribution and properties; solution of Schroedinger equation in the mean-field approximation, with atomic expansion of molecular orbitals
Ab initio and DFT calculations with periodic boundary conditions
Polarizable Continuum Model (PCM) for the simulation of solvent effects on molecular structures and energies

Simulation software and type of numerics used
Computational packages:

Gaussian03, Turbomole 6.0 for DFT
Crystal06 (for DFT with periodic boundary conditions)
Gaussian03(for PCM)
SCF Self-consistent differential equations for solvent effects with PCM
MSINW07

Achievements of the model beyond experiments
Trial and error synthesis costs were avoided by computing the energetics of inclusion of some anions (iodide and tri-iodide) in a layered solid analogous to hydrotalcite before the actual systems were synthesized. The calculations showed the limit concentration expected for anions in this environment.
The models could provide understanding of phenomena occurring, e.g. the excess of lead observed in certain conditions.
The calculations allowed to predict which surface passivant would help obtain particles of octahedral shape exposing (111) crystallographic faces, and this will guide the experiments.

Application
Solar cells

Relevant review articles:
Simona Fantacci, Filippo De Angelis "A computational approach to the electronic and optical properties of Ru(II) and Ir(III) polypyridyl complexes: Applications to DSC, OLED and NLO", Coordination Chemistry Reviews 255 (2011) 2704–2726
Walter R. Duncan and Oleg V. Prezhdo "Theoretical Studies of Photoinduced Electron Transfer in Dye-Sensitized TiO2", Annu. Rev. Phys. Chem. 58 (2007) 143–184

Summary of the project

INNOVASOL aims at developing nanostructured and molecular materials for photovoltaic (PV) excitonic solar cells. The first step is the substitution of the liquid electrolytes, currently used in dye-sensitised solar cells, with solid-state hole conductors. In parallel, semiconductor quantum dots (QDs) with tuned band gap, designed to enhance the photon capture efficiency, will replace the organic dyes as light absorbers.

Summary of the modelling

Most modelling results have been obtained with DFT with hybrid GGA functionals, though also Hartree-Fock and post-Hartree-Fock calculations have been performed. In some cases, periodic boundary conditions have been used; both finite cluster and infinite periodic models made use of Gaussian-type atomic orbitals to expand the molecular orbitals. The packages adopted were Gaussian03 and Turbomole 6.0 for finite cluster models and Crystal06 for periodic systems. When necessary, the solvent effects were included in the calculations through the Polarizable Continuum Model, where the solvent reaction field is simulated by a set of apparent charges self-consistently determined on the basis of the electric potential generated by the solvated molecule(s). This approach, partially developed in the past by some participants to the project is presently implemented in several codes: during INNOVASOL the implementation in Gaussian03 was used.
In addition to ab initio and DFT methods, also semi-empirical programs were used to describe at a lower level the effect of surrounding micro-systems, weakly interacting with the molecules. The adopted semi-empirical method was MSINDO7, with some adjustment of the parameters to fit model post-HF calculations.
Suitable meta-procedures were developed to link DFT and semi-empirical calculations in an ONIOM-like scheme (in which the more expensive DFT calculations are limited to the central molecules, whose properties are to be determined accurately, while the cheaper semi-empirical approach is used to include at a lower level the interactions with the surroundings). Routines to link MSINDO7 and Gaussian03 codes were written.
The formation energy of some inclusion complexes in layered magnesium oxides (HTLC) which is relevant for the synthesis of quasi-solid electrolytes to be used in solar cells was simulated. Also PbSe nanoparticles were modeled, with particular attention to the binding energy of the different crystallographic faces to organic passivants, and the simulation of organic dyes/PbSe nanoparticles adducts.

In summary, computational tools proved to be efficient and useful in the following project achievements.
- Limit concentration and best choice of reaction partners were predicted for the synthesis of quasi-solid electrolytes by means of ab initio periodic calculations.
- Structural properties of PbSe nanoclusters and best affinities of clusters for different organic ligands used in syntheses were computed with ab initio finite cluster approach.
- Light absorption spectra of squaraine molecules in different conditions (isolated, dissolved in liquid media, attached on top of nanoparticles) were computed with time-dependent DFT methods including solvent effects via PCM, indicating which anchoring groups are more promising for adding the dye to the nanoparticles, and how the absorption spectra can change upon addition.
- The structure of dye monolayers on TiO2 surfaces has been described with mixed ab initio – semi-empirical calculations, to estimate the binding energy as a function of anchoring groups and degree of surface coverage, i. e. the limit concentration of adsorbed dye.

http:// www.innovasol.eu

Project Acronym and Number: INNOVASOL 227057
Project Title: Innovative Materials for Future Generation Excitonic Solar Cells
Start and End Dates: 01/04/2009 till 31/03/2012
EU Contribution: 2.899.510 €
Coordinator: Prof. Leonardo Marchese, Dipartimento di Scienze e Innovazione Tecnologica, Università degli Studi del Piemonte Orientale "A. Avogadro", Italy, leonardo.marchese@mfn.unipm.it

Modelling

in IRON-SEA 283141

Subject of the modelling
Fe-based superconductors
Characteristics of Josephson junctions (junctions where a supercurrent can flow through a non superconducting medium between two superconductors)

Models used
Multiband Eliashberg models (development and application)
Blonder-Tinkham-Klapwijk model (application and extensions)
RCSJ (resistively and capacitively shunted junction) model (application)

Simulation software and type of numerics used
Systems of non linear singular integral equations solved numerically by using in-house developed code.
Systems of second-order differential equations where standard solvers are used (i.e. Runge-Kutta)
Elk code for the calculation of band-structure and Fermi surface.

Achievements of the model beyond experiments
The model determined the pairing symmetry and its evolution with doping, which is impossible to determine experimentally.
The model determined the characteristic energy of the boson that mediates superconductivity (examples: Co-doped Ba-122, Sm-1111) and of the coupling strength.
The model determined the effects of disorder, doping, lattice strain, etc on the superconducting properties.
The model determined the effects that are optimal or detrimental for device fabrication and optimization.

Application
Superconductors

Relevant review articles
P. Seidel, Supercond. Sci. Technol. 24, 043001 (2011)
D. Daghero and R.S. Gonnelli, Supercond. Sci. Technol. 23, 043001 (2010)
D. Daghero, M. Tortello, G.A. Ummarino, and R.S. Gonnelli, Rep. Prog. Phys. 74, 124509 (2011)
G.A. Ummarino, Physical Review B 83, 092508 (2011).
P. Popovich, A.V. Boris, O.V. Dolgov, A.A. Golubov, D.L. Sun, C.T. Lin, R.K. Kremer, and B. Keimer, Phys. Rev. Lett. 105, 027003 (2010)

Summary of the project

The project will study iron-based superconductors in the form of thin films, which have been prepared by molecular beam epitaxy and by pulsed laser deposition. The goal is to find unique physical properties, which lead to exploring new kinds of devices and applications. Since the iron-based superconductors have a multi-band nature, comparative studies to MgB2, which is a two-band superconductor, are also carried out.

Summary of the modelling

Intrinsic physical parameters (e.g. the superconducting transition temperature, the penetration depth, the upper critical field, and etc.) of Fe-based superconductors can be calculated by solving the three or four band Eliashberg equation, once the relevant Eliashberg parameters for a given materials are fixed. The Eliashberg theory allows calculating many different observables related to the superconducting state. In Fe-based superconductors, the solution of multiband Eliashberg equations requires some input parameters that can be either determined experimentally or provided by electronic structure calculations. Some very basic parameters related to the superconducting state can be adjusted to reproduce given experimental results. After that, it is possible to calculate with the same parameters and no further assumptions many different observables that can then be compared to experimental results or trigger new experiments to test the predictions. The analysis of a given material within the multiband Eliashberg models, especially when it is possible to explore the phase diagram can help discriminating between the effects of disorder, lattice parameters, changes in the density of states in determining the critical temperature or other superconducting properties. This can help optimizing the quality of the samples or even suggest some alternative chemical compositions or substrates (in the case of films).
Conductance-Voltage characteristics of Fe-based superconducting films obtained from point contact Andreev reflection spectroscopy measurements will be fitted to extract the superconducting energy gaps by means of the Blonder-Tinkam Klapwijk (BTK) model and its generalizations, for example to account for the real shape of the Fermi surface.
Characteristics of Josephson junctions fabricated from Fe-based superconducting films can be described by the resistively and capacitively shunted junction (RSCJ) model.
These models (BTK and its generalizations and RSCJ) are intrinsically aimed at explaining / fitting experimental data. Some of the parameters that can be extracted from the fit are specific of the single junction or point contact. Others can be compared to the outcomes of other measurements (specific heat, superfluid density, ARPES and so on). In most cases, the results for a specific material turn out to be in good agreement with those provided by these other techniques.
Theoretical aspects of the tunnelling and Andreev reflection in unconventional superconductors will be studied. In particular, they shall concentrate on:
- the Josephson effect and its dependence on the pairing symmetry
- the possibilities to use the Josephson effect to gain insight into deviations from the standard BCS -like behaviour.
- the analysis of the results of the different spectroscopy measurements in the framework of multiband Eliashberg theory with the main purpose of shedding light on the pairing mechanism and the nature of the mediating boson in Fe-based superconductors.

http://www.IronSea.eu

Project Acronym and Number: IRON-SEA 283141
Project Title: Establishing the basic science and technology for Iron-based superconducting electronics applications
Start and End Dates: 01/10/2011 till 30/09/2014
EU Contribution: 1.665.611 €
Coordinator: Kazumasa Iida, IFW, Dresden,Germany k.iida@ifw-dresden.de

Modelling

in LEMSUPER 283214

Subject of the modelling

Light element superconductivity

Models used

Molecular models for interactions, vibron properties, Jahn Teller effects
DFT for electronic structure of relevant materials
Ab initio molecular dynamics models for pressure induced metallization of potential high pressure superconductors
Advanced mean-field study of correlation effects on the ground state properties of relevant materials
Tight binding (TB) and Hubbard models built by direct inspection or by downfolding DFT electronic structure as relevant for actual or potential superconductors
Anderson impurity models and Kondo models representing a strongly interacting molecule or cluster of molecules embedded in a Fermi sea.

Simulation software and type of numerics used

Exact diagonalization, Born-Oppenheimer and similar calculations of molecular states
Solution of Kohn-Sham and related equations for standard DFT calculations and simulations with a variety of hybrid functionals (HSE, B3LYP) and LDA+U
Existing Car-Parrinello-Rahman codes
Metadynamics Gutzwiller projector technique calculations for the ab-initio codes
Numerical Renormalization Group methods as appropriate for Anderson and Kondo impurity models.
Single site cellular DMFT calculations of appropriately built Hubbard models, using Anderson model methods as an ingredient

Achievements of the model beyond experiments

New correlation-driven mechanisms for superconductivity in light element systems were predicted long before they were validated. A superconductivity mechanism for fullerides was predicted, where electron-vibron coupling, orbital degeneracy, and strong electron correlations implying a nearby Mott transition all play a crucial role. Cesium fullerides validated this theory.
Identification of new electronic ground states in light element systems leading to superconductivity, potentially unveiling new light element molecule-based superconductors, something that cannot be done experimentally.

Application

Light element molecules superconductors

Relevant review articles:

Capone et al. Modeling the unconventional superconducting properties of expanded A(3)C(60) fullerides 10.1103/RevModPhys.81.943 Apr-Jun 2009
Kubozono, Yoshihiro et al Metal-intercalated aromatic hydrocarbons: a new class of carbon-based superconductors PhysChemChemPhys 13/17 2011 pp: 16476-16493 DOI: 10.1039/c1cp20961b

Summary of project

This project addresses the design and understanding of light (and cheap, abundant, benign) element (B, C, O) cluster/molecule-based superconducting systems with higher transition temperatures

Summary of the modelling

The project aims to develop new understanding of the electronic and crystal structures required for high Tc superconductivity in light element systems. Competing electronic ground states and pairing mechanisms are at the basis of superconductivity. In light element materials a fine balance exists between electron-phonon coupling and the electron correlations. This was recently identified as the potential of light elements as superconductors.
In light elements superconductivity is controlled by p orbitals and the π-orbitals of C contribute to the LUMO (lowest unoccupied molecular orbital, filled by the electrons donated by the alkali dopants). Furthermore the Coulomb exchange interaction play a role, and the C-C phonon modes bring about the molecular vibrations relevant for superconductivity. Alkali doped fullerenes, fullerides and polycyclic aromatic hydrocarbons near metal-insulator transitions, where they are likely to develop superconductivity, will be studied. Also the influence of external actions, such as doping, pressure, electric fields will be investigated. The simultaneous role of correlations, screening and disorder will be considered, with special attention to the role that disorder may play in enhancing the critical temperature at the transition.
The electronic structure, magnetism, phonon structure will be obtained by density functional theory (DFT) calculations, even in strongly correlated systems. Insulating or metallic tendencies and the Fermi surfaces of candidate light element and molecular superconductors can be addressed with an initial DFT study. The DFT total energies and enthalpies generally provide a good indication of the relative stability of different crystal structures. Relativistic effects, including Rashba at interfaces, can automatically be included by means of DFT codes including spin orbit. The electron phonon couplings, key ingredients to BCS superconductivity in regular metals and also in Jahn Teller systems, can be reasonably obtained by DFT. In addition correlations can be built-in at the mean-field level through approximations such as LDA+U or equivalent. DFT with a variety of hybrid functionals (HSE, B3LYP) and LDA+U models will be applied to identify aromatic superconductor materials that show a conduction band which comprises multibands and a Fermi surface which is an interesting composite of surfaces having different spatial dimensionalities.
Full many-body models such as Dynamical Mean Field Theory (DMFT) with the "downfolding" description of the Mott-Hubbard insulator will also be applied.
Many body techniques for metal-insulator interfaces able to describe inhomogeneous situations will be developed for application to surface doping. The effect of many body interactions beyond mean-field levels in picene and similar molecular systems will be added to the models. The models will then be available for materials exploration of the rich variety in molecular species (various aromatic molecules in the present project), orbitals and crystal structures in order to find materials with long-ranged electron-electron interaction, expected to substantially affect the mechanism of superconductivity.
The superconductor- insulator transition in lattice expanded alkali fullerides has properties not yet experimentally explored. Insulator-superconductor transitions obtainable under pressure and/or in other organic doped systems will be investigated to identify materials that are possible candidates.

http://www.lemsuper.eu

Project Acronym and Number: LEMSUPER 283214
Project Title: Light element molecular superconductivity and interdisciplinary approach
Start and End Dates: 01/10/2011 till 31/03/2015
EU Contribution: 1.606.660 €
Coordinator: E. Tosatti, SISSA, Trieste, Italy; tosatti@sissa.it

Modelling

in MAGNONICS 228673

Subject of the modelling

Nanostructured magnetic (magnonic) metamaterials with GHz and THz dynamics and/or with unusual electromagnetic properties (negative permeability in certain frequency ranges, band gaps in magnonic dispersion etc).

Models used

Electromagnetic and spin dynamics models for calculating band gap and effectively continuous properties describing excitations in magnonic metamaterials consisting of patterned magnetic nanoelements:

- Finite-difference (MicroMagus, OOMMF) and finite-element (Nmag) micromagnetic simulations based on the Landau-Lifshitz equation for computing magnetization dynamics in the time-domain
- Plane wave method (PWM) for the calculation of magnonic spectra
- Dynamical matrix method for dipole-coupled magnetic nanoelements and arrays of antidots
- Simulations of ordered and disordered systems of single-domain fine magnetic particles taking into account the magnetodipolar interparticle interaction
- MatLab based solution of full Maxwell equations with account of ferromagnetic resonance phenomena

Simulation software and type of numerics used

Finite difference modelling (both micromagnetics and based on full Maxwell equations)
Finite-element modeling (micromagnetics)
Matrix diagonalization

Achievements of the model beyond experiments

Numerical simulation of quasistatic magnetization processes explain measurements by MOKE and of spin-wave excitations observed by FMR, BLS, and TRSKM techniques in 2D arrays of nanoscale magnetic dots and antidots. These simulations facilitate explaining the nature and spatial structure of magnons in the magnonic arrays.

Application

Electromagnetic antennas (e.g. patch antennas), and signal conditioning devices (e.g. microwave filters); magnonic devices and logic architectures, including magnonic filters, logic gates, programmable gate arrays.

Relevant review articles

V. V. Kruglyak, S. O. Demokritov, and D. Grundler, “Magnonics”, J. Phys. D – Appl. Phys. 43, 264001 (2010); S. - K. Kim, “Micromagnetic computer simulations of spin waves in nanometre-scale patterned magnetic elements”, J. Phys. D – Appl. Phys. 43, 264004 (2010).

Summary of the project

The project aims at creation of materials with artificial structures - so called metamaterials – having the GHz and THz excitation spectra with prescribed features (peaks and band gaps in given frequency regions). With respect to long wavelength spin waves, the artificial nanostructures will behave as effectively uniform and have effectively continuous magnetic properties not seen in nature. For short wavelengths the material will show band gaps.

Summary of the modelling

MAGNONICS focussed on the comprehensive theoretical understanding of the band gap and effectively continuous properties of the created magnonic metamaterials.

The plane wave method (PWM) has been used for the calculation of magnonic band structure of thin slabs of 1D and 2D magnonic crystals and validated via comparison with experimental results.

The PWM has been applied to the calculation of magnonic spectra of antidot lattices and used to interpret experimental data acquired using broadband microwave spectroscopy and BLS.

The dynamical matrix method has been used to deal with dipole-coupled nanoelements and arrays of antidots and to evaluate the BLS cross section. It has been applied to systems experimentally investigated within the project: chains and 2D arrays of magnetic dots, square arrays of antidots.

Thermally excited spin waves in planar one- and two-dimensional magnonic crystals have been studied using both conventional (k-vector resolved) and micro-focused (spatial resolved) BLS measurements in arrays of dense magnetic elements (dots and stripes) and antidots (periodic arrangement of holes embedded into a continuous magnetic film), and the results have been compared with calculations performed by micromagnetic simulations, the PWM, and the DMM.

The 3-dimensional (3D) version of the Fast Fourier technique (FFT) for calculating the magneto-dipolar interaction field in continuous ferromagnetic structures has been implemented, so that large-scale simulations of 3D micromagnetic problems have become possible.

The combined Ewald-FFT method for the calculation of the magneto-dipole interaction field in ordered and disordered systems of fine magnetic particles has been applied. In particular, this method enables highly efficient numerical simulations of magnetization processes in magneto-ferritin-based crystals.

Numerical simulation of quasi-static magnetization processes measured by MOKE and of spin-wave excitations observed by FMR, BLS, and TRSKM techniques in 2D arrays of magnetic nanodots have been performed. These simulations allow to explain the nature and to find out the spatial structure of corresponding magnons in the nanodot arrays under study.

www.magnonics.org

Project Acronym and Number: MAGNONICS 228673
Project Title: MAGNONICS: Mastering Magnons in Magnetic Meta-Materials
Start and End Dates: 15/09/2009 till 14/09/2012
EU Contribution: 3.499.820 €
Coordinator: Volodymyr Kruglyak, University of Exeter, UK, V.V.Kruglyak@exeter.ac.uk

Modelling

in MASTER 212257

Subject of the modelling

Spin wave excitation by spin-polarized current and spin-diffusion effect in normal metal near a junction

Models used

Micromagnetic model (Landau Lifshitz Gilbert equation)

Simulation software and type of numerics used

Micromagnetic package SpinPM, a generalized Landau Lifshitz Gilbert solver based on 4th order Runge-Kutta scheme with INTEL MKL FFT acceleration. It integrates:

- Plug&Play user-friendly GUI
- FFT-accelerated magnetostatics
- time integration using 4th order Runge-Kutta solver
- time step auto-adaptation
- very flexible system definition
- Spin Transfer Torque with both Slonczewski and Field-like torques

Achievements of the model beyond experiments

The model can predict the magnetization dynamics in an array of hetero-structures. These dynamics cannot be computed analytically. These simulations are used to optimize the design of spin devices as optimization by experimental means would be too costly.

Application

Mobile and wireless telecommunication technology
Spin torque devices

Relevant review articles

A.V. Khvalkovskiy, KAZ, et al Phys. Rev. B. 80, 140401(R), (2009)
A. Chanthbouala, AVKh, KAZ, et al., Nature Physics 7, 626 (2011)
A. Dussaux, AVKh, KAZ et al., Nature Com. 1, 1 (2010)
A.D.Belanovsky, KAZ, et al, Phys. Rev. B 85, 100409(R), (2012)

Summary of the project

MASTER is to explore microwave signal generation for integrated microwave components and wireless communications systems. The so-called Spin Transfer Nano-Oscillator (or STNO), can provide solutions to miniturization and broad-range microwave detection due to their specific spin polarized transport properties. This project aims at exploiting the coherent coupling within and between devices developed in large array to improve the microwave performances in terms of phase noise, emission power and to operate in different frequency ranges.

Summary of the modelling

The application of existing micromagnetic packages allowed us to reveal the influence of geometry and structural defects upon the STO phase diagram, phase-locking performance, and line width, and to create a virtual prototype of the STO array with optimized properties. The role of the thermal fluctuations in the phase-locking mechanism has also been investigated within the framework of a full scale 3D micromagnetic model, allowing the optimization of the array. Magnetization dynamics have been investigated in polycrystalline films, with the parameters of magnetic materials being distributed randomly over the crystallites. The model has been elaborated with the Berger / Slonczewski transport term. The code SpinPM simulates spin current-related effects and an extension that includes spin transfer-induced torque has been developed.

The project also developed a simple theoretical framework for transport in magnetic multilayers, based on the Landauer-Büttiker scattering formalism and random matrix theory. A simple transformation allows one to go from the scattering point of view to theories expressed in terms of local currents and the electromagnetic potential. In particular, the theory can be mapped onto the well-established classical Valet-Fert theory for collinear systems. The scattering formalism as our starting point and develop a theory which fully captures Valet-Fert and (generalized) circuit theory. The theory, referred to as C-RMT (for Continuous Random Matrix Theory), can be tabulated by the same set of (experimentally accessible) parameters as Valet-Fert. C-RMT will be included in the micromagnetic solver.

The projects also enhanced the micromagnetic numerical solver.The code has been elaborated to be able to deal with high simulation volume (up to few micrometer big lateral sizes), non-regular structure (multilayered structures), non-regular dynamics (very short-wavelength modes are excited), and huge computational times (> 50 ns). Features to define the structures and to help the analysis of the magnetization dynamics of the system have been added. The most important improvements in the software SpinPM are:
New time integration algorithm based on an integration procedure that includes an adaptive time-step control with a 4th order Runge-Kutta method
New exchange energy calculation algorithm: a new, energy-conserving, numerical algorithm has been developed and implemented allowing very simulations on very long time range
Fine system specification allowing much better flexibility in object specification
Spectra calculations: This tool provides us with a possibility to calculate these spectra for a batch of projects

http://iramis.cea.fr/spec/Phocea/Page/index.php?id=23

Project Acronym and Number: MASTER 212257
Project Title: Microwave Amplification by Spin Transfer Emission Radiation
Start and End Dates: 01/09/2008 till 29/02/2012
EU Contribution: 2,044,210 €
Coordinator: Olivier Klein, CEA, FR olivier.klein@cea.fr

Modelling

in MATRANS 228869

Subject of the modelling

Properties and behaviour of metal-ceramic functionally graded materials (FGM) (alumina ceramics and copper or Ni-Al intermetallics) at the stage of processing and under service conditions

Models used

- Continuum mechanics models with phenomenological constitutive equations for materials behaviour (processing induced thermal residual stresses and material damage; static and dynamic fracture; thermomechanical fatigue)
- Continuum micromechanical models (effective thermomechanical properties; design of material macro-properties by modelling; modelling of wear, including shape evolution and coupling with oxidation)

Simulation software and type of numerics used

Abaqus, ANSYS AceFEM and FEAP for solid mechanics

FE^2 for multi-scale thermomechanics modeling

Numerics

Finite elements with three dimensional automatic mesh generation (e.g. SCAN/IP SCAN/FE) coupled with micro-tomography digital images of real material microstructures

Automation of finite element computations using symbolic algebra software (e.g. AceFEM)

self-consistent method or the Mori-Tanaka method

Multi-objective optimisation method to find the optimal composition

Achievements of the model beyond experiments

Most of the modelling in the project is done to replace the experiments, which are usually complex and costly or, in other words, the modelling predicts the materials' properties/behaviour which will be observed in experiments and thus shortens the development process.

Application

- Transport (aerospace and automotive), Energy

Relevant review articles

Y.C. Fung and Pin Tong. Classical and Computational Solid Mechanics, World Scientific, 2001.

P. Wriggers. Computational Contact Mechanics, Springer-Verlag, Berlin Heidelberg 2006.

G.W. Stachowiak (ed.). Wear - Materials, Mechanisms and Practice, John Wiley and Sons 2006.

R.M. Christensen. Mechanics of Composite Materials. Dover Publications, Mineola, New York 2005.

M.F. Ashby. Material selection in mechanical design, 4-th edition. Butterworth-Heinemann, Amsterdam 2011.

J. LLorca. Fatigue of particle-and whisker-reinforced metal-matrix composites. *Progress in Materials Science,* 2002 *(*47), 283

P.N. Bogdanovich, D.V. Tkachuk. Thermal and Thermomechanical Phenomena in Sliding Contact. Journal of Friction and Wear, 2009 (30), 153–163.

G.A. Maugin, Configurational Forces: Thermomechanics, physics, mathematics, and numerics. Taylor & Francis, NY, 2011.

S. Murakami, Continuum Damage Mechanics: A Continuum Mechanics Approach to the Analysis of Damage and Fracture. Springer, 2012.

L. Mishnaevsky Jr., Computational Mesomechanics of Composites, Wiley, England, 2007.

Summary of the project

MATRANS aims at developing novel metal-ceramic functionally graded materials (FGMs) for aerospace and automotive applications in exhaust and propulsion systems (e.g. thruster), power transmission systems (e.g. valves), and braking systems. The main objective is to enhance the mechanical properties of these materials through spatial variations of material composition and microstructure.

Summary of the modelling

Modelling of graded profile of FGMs (i.e. number of layers, their arrangement and volume fraction of metal and ceramic phases in individual layers) was approached as a transient thermo-mechanical problem of continuum mechanics with account of deformation and damage evolution depending on structural parameters variation.

Physical quantities involved in this analysis include temperature, stress, strain, yield and crack resistivity. The sample is subjected to different temperatures and mechanical loadings. As the outcome we obtain stress, strain and optimal ceramic phase distribution in the sample. The software used for numerical solution was AceFEM - a general finite element system for Mathematica, combining symbolic and numeric approaches.

The effective linear thermoelastic properties of the FGM constituent layers were modeled using the full set of conservation principles along with the constitutive equations that relate the mechanical and thermal properties of the individual (metal and ceramic) solid phases. Macroscopic properties of the heterogeneous material were derived from the phase and morphology data either analytically or numerically by using homogenisation techniques such as the self-consistent method or the Mori-Tanaka method.

To model nonlinear overall properties, the above micromechanical approaches were extended to a sequence of incremental problems, linearized using either tangent or secant stiffness moduli, and implemented numerically within the Mathematica package.

Calculated macroscopic properties depend strongly on the material composition. An optimal content of the ceramic phase was searched for, which would meet the required thermo-mechanical properties of the composite for the target applications. For this purpose, a multi-objective optimization problem of continuum thermomechanics was formulated and solved numerically. The relevant objective function expresses the distance between required effective properties and their micromechanical estimates.

Several existing constitutive models have been coupled in such a way as to assist in revealing the influence of various micro defects (pores, matrix cracks, debonding cracks at interfaces between matrix and inclusions) introduced during the manufacture of metal-ceramic functionally graded materials on their macroscopic properties. These models have been validated on Cu-Al_2O_3 metal-matrix composites and implemented as an external module in the commercial finite element code Abaqus.

A continuum model to calculate thermal residual stresses and damage in graded metal-ceramic composites, generated during the cooling phase of the sintering process, was developed and implemented numerically with FEM, making use of microstructural material data from micro-CT images and transforming it onto finite elements by means of SCAN/IP and SCAN/FE software. The material models used in the FEM computations are the three conservation equations with a linear elastic constitutive equation for the ceramic and an elasto-plastic constitutive equation for the metal phase. Numerical calculations of thermal residual stresses and the resulting material damage were done using FEAP and Abaqus programmes.

Processing-induced microcracking in metal-ceramic composites due to mismatch of thermal properties of the constituent materials was calculated by micromechanical models with configurational forces considered to be the driving forces of macroscopic cracks and defects. The parameters of the macroscopic constitutive equations were either obtained by measurements or by micromechanical modelling. The micromechanical models were solved on a grid of voxels representing either the metal or the ceramics phase of the composite with the microstructural data coming from micro-CT scans or from a randomly generated

microstructure. A voxel based generation of three dimensional FE models based on Mishnaevsky (2007) numerical procedures was used in the computations.

A phenomenological model of contact wear has been formulated which provides a constitutive equation relating the local wear rate (wear volume per unit area and per unit time) to contact variables (contact pressure, sliding velocity, etc.) and material properties (e.g. hardness, composition of an FGM layer, etc.). The model is a generalization of the classical Archard wear model. The wear model is a part of the contact and wear problem in which the equilibrium equations (balance of linear momentum) are solved on a varying domain, and the evolution of the domain is determined by the wear model. Thus two problems are solved simultaneously: the deformation (contact) problem and the shape evolution problem. The main focus of the work is on development of a solution strategy based on an unconditionally stable implicit time integration scheme and on development implementation of efficient computational algorithms suitable for this class of problems. The finite element implementation and the computations are performed using the AceGen/AceFEM system. Efficient computational algorithms have been developed which are not part of the existing commercial FEM codes.

A phenomenological model of oxidation coupled with wear was proposed for the alumina-copper FGM developed for the brake disk application. The model gives the oxide mass evolution (the wear and oxide change rates) as function of temperature, contact stress and time. The model is based on experimental observations from Thermo-Gravimetric Analysis (TGA) at a given temperature, tribological wear test (ball on disk) and real surface topography measurement. The wear-oxidation process was solved using a two scale approach. The first scale is the macroscopic level, corresponding e.g. to the ball on disc test of a braking system, the second scale is the asperity microscale level. On the microscale Finite Element Analysis with thermo-mechanical coupling was used for the calculation of averaged wear-oxidation parameters. Finally, on the macroscale the evolution of shape, stress and temperature (affected by the wear-oxidation processes) was calculated using FEM (Abaqus).

Models of mechanical and thermal fatigue of the copper-alumina FGM intended for the thruster application were developed using micromechanical and continuum mechanics approaches. The low-cycle fatigue behaviour of composite is treated as a localized damage development phenomenon activated by applied cyclic loading. The modelling is based in part on the analytical analysis on the microscale of the representative cell, formed by a composite element of a specified size and particle volume ratio. The energy equations are formulated to describe the energy balance with account for the stress transfer between the brittle-particles and ductile-matrix with different possible scenarios of damage localisation. On the macroscale the numerical analysis by the FEM (Abaqus) is used in which the representative damage parameter is introduced affecting the stiffness moduli of the macro element. The predictive result of these models is a relationship between the number of loading cycles (fatigue life) and the critical stress/accumulated equivalent plastic strain sustained by the material.

A series of fully coupled linear thermoelastic models of brake disk demonstrator solved with FE techniques were developed and tested. The focus was on the optimal design of the brake disk and on simulation of mechanical strength. The effective material properties were used as input in phenomenological model.

A new constitutive model defining the relationship between tensile strength of functionally graded materials (FGMs) and volume fraction of ceramic phase has been developed to simplify complicated mechanical behaviour of FGMs.

In oxidation modelling a new constitutive relation has been proposed between the oxide growth rate and the surface temperature. Since the calculated macro temperatures are too low to allow for the oxidation, only closer look at surface asperities can provide the mathematical model for the experimentally observed oxidation phenomena. A user-defined FORTRAN code for the developed constitutive relation has been added to a commercial FE software.

matrans.kmm-vin.eu

Project Acronym and Number: MATRANS 228869
Project Title: Micro and Nanocrystalline Functionally Graded Materials for Transport Applications
Start and End Dates: 01/02/2010 till 31/01/2013
EU Contribution: 3.600.000 €
Coordinator: Michal Basista, KMM-VIN AISBL, Michal.Basista@kmm-vin.eu

Modelling

in METACHEM 228762

Subject of the modelling

Characterisation of electro-magnetic properties of thin-film metamaterials with well-defined boundaries

Extraction of optical constants from measured optical data (variable angle spectroscopic ellipsometry, transmission, reflection, phase.)

Models used

Maxwell equations with boundary conditions and different types of sources (plane wave; wave port; Gaussian beam; point dipole, etc)

Models developed for extraction of bulk properties of the materials (mainly real and imaginary parts of permittivity)

Generalized Mie Model (GMM) of scattering by clusters of simple and core-shell spheres

Simulation software and type of numerics used

Ansoft HFSS

CST Studio Suite

Original analytical method of dynamic homogenization for so-called Bloch lattices

Original analytical method of dynamic homogenization for so-called metasurfaces

Fresnel modelling using commercial WVASE software, a corrected Sivukhin-Debye model

Integral equation approach and discretization of the surfaces with the help of GMSH,

Accelerations:

- Exponentially converging (and tabulated) periodic Green's functions.
- Compression of matrix of system of equations using the incomplete-QR approach
- Matrix reduction using multiple-scattering Macro Basis Functions

Achievements of the model beyond experiments

The model predicts whether the metamaterial can be described within effective media theory.

The model extracts parameters not directly measurable.

The model can determine individual polarizabilities of a complex scatterer (electric and magnetic), surface susceptibilities of metasurfaces (electric, magnetic and magnetoelectric), refractive index of the wave in a lattice and wave impedance of the wave in a lattice.

Application

Optical devices

Characterization of metamaterials

Relevant review articles

http://ec.europa.eu/research/industrial_technologies/pdf/metamaterials-brochure_en.pdf

Summary of the project

The objective of the METACHEM collaborative project is to use the extreme versatility of nanochemistry and the physical-chemistry routes of self-assembly to design and manufacture bulk meta-materials exhibiting non-conventional electromagnetic properties in the range of visible light.

Summary of the modelling

EM theory and numerical simulations provide guidance for designs by calculating which materials, shape of particles and range of sizes can provide new metamaterial properties. The aim is also to understand the consequences of disorder (in size and position). The models will give the effective optical parameters of the metamaterial (refractive indices, thickness, bi-anisotropy, etc.).

Plane wave models are used for the extraction of bulk properties of the materials (mainly real and imaginary parts of permittivity).

The generalized Mie Model (GMM) is used to study scattering by clusters of simple and core-shell spheres and also for the study of gain media, in combination with appropriate periodic Green's functions.

Ansoft HFSS and CST Studio Suite are used for infinite-array simulations of periodic meta-volumes and meta-surfaces in combination with plane-wave models (see above) for the extraction of material parameters.

Integral-equation approaches are used for the accelerated analysis of large finite structures and structures made of complex inclusions (systematic reduction of complexity with "macro basis functions"). It easily allows for the computation of "point spread functions" (response of a metamaterial to a nearby localized source). This approach is used for fast infinite-array response of magnetic nano-particles, point-spread function of arrays of nanorods, and study of disorder in large finite arrays.

The transmission, reflection and ellipsometry spectra measured at different angles of incidence (ellipsometric data) are used to extract values of optical constants of metamaterial. The spectroscopic data will be also analyzed with the help of the Sivukhin-Debye approach, which has a much better accuracy than effective medium theories in case of small film thickness.

https://www.metachem-fp7.eu/

Project Acronym and Number: METACHEM 228762
Project Title: Nanochemistry and self-assembly routes to metamaterials for visible light
Start and End Dates: 15/09/2009 till 15/09/2013
EU Contribution: 3.499.820 €
Coordinator: Philippe Barois, CNRS-Bordeaux, FR, barois@crpp-bordeaux.cnrs.fr

Modelling

in MINOTOR 228424

Subject of the modelling

Electronic phenomena at interfaces in organic-based electronic devices

Models used

Ab initio or semi-empirical Hartree-Fock methods, DFT methods, Molecular Dynamics, QM/MM, Monte Carlo algorithms, classical microelectrostatic models

Software code and type of numerics used

Gaussian, Ampac, Fireball, VASP, SIESTA, Gromacs, Materials Studio, Tinker, NAMD

Achievements of the model beyond experiments

Modelling allows material design of multilayer devices with optimized proprieties as follows:

- The model has predicted the contributions to the discontinuity between the electronic structure at the interface and the bulk material
- The model explained the origin of the electronic level alignments at organic/organic interfaces as measured in short-circuit current and the open circuit voltage of solar cell devices, two key quantities that directly dictate the efficiency of those cells.
- The model has shown that modifying the surface of electrodes, can tune the charge or spin injection barriers in devices such as OLEDs.
- The model predicted the influence of lattice mismatches at the interface between two crystalline organic semi-conductors on the interfacial electronic properties.

Application

OLEDs, transistors, sensors and storage devices, solar cells

Relevant review articles

"Electronic structure and geminate pair energetics at organic - organic interfaces: the case of pentacene/ C60 heterojunctions". S.Verlaak, D.Beljonne, D.Cheyns, C.Rolin, M.Linares, F.Castet, J.Cornil and P.Heremans. Advanced Functional Materials 2009, 19, 3809-3814
"Electronic Processes at Organic-Organic Interfaces: Insight from Modeling and Implications for Opto-Electronic Devices". D.Beljonne, J.Cornil, L.Muccioli, C.Zannoni, J.L.Brédas and F.Castet. Chemistry of materials 2011, 23, 591-609
"Barrier Height formation for the PTCDA/Au (111) interface" J.I.Martinez, E.Abad, F.Flores, J.Ortega, G.Brocks Chemical Physics, 2011, 390, 14-19.

Summary of the project

The main goal of MINOTOR is to develop a multiscale theoretical approach to model the interfaces in organic-based electronic devices and the electronic phenomena taking place at these interfaces in order to optimize the device efficiency. Organic electronics and spin-based electronics use organic conjugated molecules and polymers in multi-layer devices. Many key electronic processes (such as charge injection from metallic electrodes, charge recombination into light or light conversion into charges, spin injection, etc.) occur at interfaces and predictive models need to be developed to reproduce and fine tune new materials characteristics.

Summary of the modeling

The project applied modelling approaches to investigate electronic and structural properties at organic-organic, organic-metal, and organic-inorganic interfaces, in close conjunction with corresponding experimental measurements.
MINOTOR aimed at a multi-scale modelling approach ranging from the atomistic to the mesoscopic scale. In particular, the modelling could predict and explain:

- Changes in the work function of metal electrodes upon deposition of self-assembled monolayers or organic semiconductors using DFT calculations with Periodic Boundary Conditions (as implemented in VASP, SIESTA, FIREBALL)
- The nature of interface dipoles formed at organic/organic interfaces by modelling the morphology at the atomistic level with Molecular Dynamics simulations and by computing the electronic properties of model systems or aggregates extracted from the MD snapshots using semi-empirical Hartree-Fock techniques or DFT calculations validated against highly correlated CASSCF and MP2 approaches.
- The nature of the dipoles at interfaces between organic semiconductors and oxide layers (ZnO, TiO2) and the resulting shift in the workfunction of the oxide layer at the DFT and tight-binding DFT levels; realistic morphologies have also been generated at the MD level.
- The mechanism of free charge carrier generation in organic solar cells by computing the energetic profile of the charge carriers around the interface with a classical microelectrostatic model with all relevant parameters provided by quantum-chemical calculations.
- The mechanism of chemical doping of organic layers to yield enhanced conductivities by determining the energy landscape of the charge carriers with a classical microelectrostatic model; in a next step, the charge carriers are propagated in the doped layer by means of Monte-Carlo simulations relying on hopping transfer rates (with all molecular ingredients provided by quantum-chemical calculations and the energetic disorder by the microelectrostatic model) in order to evaluate the density of free carriers.

http://www.materianova.be/minotor

Project Acronym and Number: MINOTOR 228424
Project Title: Modelling of electronic processes at interfaces in organic-based electronic devices
Start and End Dates: 01/06/2009 till 31/5/2012
EU Contribution: 3.080.098 €
Coordinator: Jerome Cornil, MONS University, Belgium, Jerome.Cornil@umons.ac.be

Modelling

in MINTWELD 229108

Subject of the modelling

Welding processes of metal alloys

Models used

Ab-initio molecular dynamics (MD) with plane wave pseudo potential
Born-Oppenheimer molecular dynamics (BOMD), classical MD simulations, by using the ab-initio fitted EAM potentials, Molecular dynamics simulation of solid-liquid interfaces with newly developed force fields.
Micro-scale Phase Field modelling
Macro-scale computational fluid dynamics modelling Thermodynamic modeling

Simulation software and type of numerics used

Quantum-Espresso software
Potfit force-matching code to fit a new EAM potential to ab-initio forces
Finite Element Analysis
Front-Tracking method
Adaptive interpolation scheme that is suitable for phase field simulations of relevant systems

Achievements of the model beyond experiments

The software predicted the failure of components under in-service loading conditions. By doing so, it accelerated the development of new welding fillers and processes and it thus reduced costs.

Application

Manufacturing industry, metal alloys, welding, EAM (electric active materials) modeling

Summary of the project

The ability to weld a metal to itself (similar welding) and to other materials (dissimilar welding) strongly depends on the chemical segregation and morphology of the advancing solidification interfaces, in particular at grain boundaries where individual crystals meet near the weld centre. The advancing solidification interfaces and the resulting grain boundaries have critical nano- and sub-micron scale features. These boundaries have different alloy concentrations due to chemical segregation during solidification, and are the regions where failure most probably occurs by cracking during solidification of the weld pool (hot cracking) or by cracking in service (cold cracking), an example is hydrogen embrittlement. Cracking is the most common failure mode in welds, and many expensive failures have occurred in welded components.
This project aims at producing an integrated suite of modelling software, with special emphasis on the solid-liquid interface evolution in industrially relevant systems, such as steel/steel and steel/nickel-based alloys.

Summary of the modelling

The computational aspects of this project aim at incorporating the realistic effects of alloy chemistry and process parameters in modelling the interface evolution during welding and the in-service failure of weld components. Multi-scale approaches which link atomistic scale ab-initio and Molecular Dynamic models (interface properties and issues of chemistry in the crack) with micro/nanoscale Phase-Field Models (grain boundary and interface chemistry and structure), and macro-scale Computational Fluid Dynamics models (heat and mass flow) are required to go beyond the current single scale model. The current challenge facing modelling of weld hot cracking is the use of existing models to describe the formation of the weld pool, the advance of the solidification interface, element segregation at the grain boundary and the influence of the welding process parameters and mechanical constraints that arise from the geometry of the work-piece. The project will use models for fluid flow, solidification, phase field and front tracking to provide thermodynamic, kinetic and element segregation information relevant to the solidification interface evolution and resulting grain boundaries. Ab-initio and molecular dynamics studies will provide surface and interface energies and develop new interatomic potentials of selected EAM. For the representation of the sample meso-scale Front-Tracking calculations (crystal growth, grain size distribution) are used.
This information will be combined within the framework of the variational principle to predict component life time.
Validation of the predictions will be ensured by novel experiments at each scale, including real-time synchrotron imaging to observe morphological evolution of the welding fronts, electron probe micro-analysis and atom probe to characterise alloy chemistry near grain boundaries.
Strategies for intelligent design of new weld materials with improved properties of the nano-organized interfaces and grain boundaries will be developed and passed on to the welding industry.
Multi-scale structure integrity analysis is taking advantage of the macro-scale CFD, meso-scale grain structure modelling, micro-scale phase field modelling and atomistic modelling to provide thermodynamic, kinetic and element segregation information relevant to the properties and failures in welded components. It is hoped that this new approach can provide us a better understanding of physical process during welding and the welded components in use.

http://www2.le.ac.uk/projects/mintweld

Project Acronym and Number: MintWeld 229108
Project Title: Modelling of Interface Evolution in Advanced Welding
Start and End Dates: 01/09/2009 till 31/08/2013
EU Contribution: 3.550.000 €
Coordinator: Prof. Hongbiao Dong, UNIVERSITY OF LEICESTER, UK, hd38@le.ac.uk

Modelling

in MODIFY 228320

Subject of the modelling
Stress-induced deformation of pressure sensitive adhesive materials (PSAs) consisting of complex formulations of acrylic polymers

Models used
All-atom molecular models and force-fields based on quantum-mechanics calculations and parameterization on the basis of experimental data.
Mesoscopic (network) model based on particle-to-particle transient forces and chain-to-chain entanglements.
Non-equilibrium thermodynamics-based theory for interfacial phenomena.
Closed-form differential constitutive equation for the rheology of highly elastic polymer-based materials, in codes for 3-d deformation of large volumes of acrylic polymers.

Simulation software and type of numerics used
Phase field formulations
LAMMPS software
Finite element code to solve the set of partial differential equations describing transport phenomena during the stretching deformation of acrylic adhesives at macro-scale accommodating several boundary conditions (slip, no-slip, generalized slip, etc).
The deformation equations were solved using (a) the mixed Galerkin/finite element method for the velocities, pressure and location of mesh nodes, and (b) the DEVSS-G with streamline upwinding method for the stress components.
Molecular structural code using the NPxxPyyPzzT statistical ensemble, where N denotes the number of interacting atomistic units in the system, Pii the normal pressure in the i-direction, and T the temperature.

Achievements of the model beyond experiments
Modelling has explained the interplay between the chemical composition of the synthesized PSA samples and the degree, strength and life-time of the specific hydrogen forces developing in the polymer, which in turn governs the unique cohesive properties and strong elasticity of these materials. Models also explained the big role played by particle-to-particle transient forces on the elasticity-to-viscosity ratio which seems to be at the heart of the design task for new adhesives. Modelling explained the connection between bulk rheological properties in extension and shear and the debonding mechanisms during stretching of PSAs.

Application
Pressure sensitive adhesive materials for cosmetics, food, paints, and coatings

Summary of the project

MODIFY has developed a hierarchical modelling framework for soft nanostructured adhesives based on acrylic polymers. These codes address a multitude of phenomena governing the performance of PSAs in real applications: cavitation, diffuse particle-particle interfaces that can transfer stress, adhesion on hard substrates and slip at high levels of stretching, elasticity-versus-viscosity, density of hydrogen bonds versus density of chain entanglements, and degree of chain cross-linking.

Summary of the modelling

The modelling framework of the MODIFY project consists of the following components:

a) The GENERIC framework of non-equilibrium thermodynamics was first utilized and extended to handle mixed systems consisting of bulk regions and interfaces based on a specific treatment of interfacial fields built on the concept of gauge invariance to atomistic displacements of the interface. The outcome of this effort has been a new type of boundary condition for elastic polymers strongly adhered on hard substrates.

b) For the solution of Hamilton's equations of motion at the atomistic level in the presence of a flow field, a generalized non-equilibrium molecular dynamics (NEMD) algorithm was developed, capable of predicting nano-scale structural changes both in the bulk of an acrylic PSA and at the interface with a substrate. The LAMMPS software was equipped with potential energy functions of relevance to the chemistry of the PSA materials.

c) Information from the atomistic simulations was used to parameterize two mesoscale models describing the bulk rheology of the model PSA systems specifically synthesized in the course of the MODIFY project for the modelling needs: one based on the Pom-Pom tube model, and a second based on a particle-based coarse-grained picture of the latex particles. The tube-based model enabled accurate empirical fits both of the linear and of the non-linear extensional rheology of the synthesized adhesives. The particle-based coarse-grained model enabled semi-quantitative predictions of their linear and non-linear rheology, using input parameters which were estimated from experiment, statistical reasoning, or more detailed (atomistic) simulations.

Constitutive equations

A macroscopic constitutive model was developed capable of describing quite reliably the deformation equations (e.g., the shear and elongational behaviour) of the synthesized PSA materials. The new equation utilizes generalized expressions for the strain energy density as a function of the three invariants of the conformation or deformation gradient tensor. In limiting cases, it reduces to known laws widely used to describe hyper-elastic materials, such as the Rivlin-Saunders and Hart-Smith theories.

Representation of the sample

An advanced geometrical code was developed to monitor moleculare structural changes upon stretching at the atomistic level; this code can compute the entanglement network, and provide information to higher-level models for the response of polymer acrylics to elongational deformation fields.

Numerics

A powerful finite-element code was developed for the full three-dimensional (3-d) simulation of the deformation of acrylic adhesives. It is based on a consistent coupling of an elliptic-mesh generation methodology with domain decomposition and local mesh refinement around deforming and moving interfaces. The transport code can follow the large adhesive and bubble deformations inside the material (which lead to fibrillation); it can also trace the elastic boundary layers that form at the moving interfaces. It can therefore reliably simulate the force-deformation history of the material under industrially relevant conditions. This is one of the biggest achievements of the MODIFY project.

http://modify.chemeng.upatras.gr/

Project Acronym and Number: MODIFY 228320
Project Title: Multi-scale modelling of interfacial phenomena in acrylic adhesives undergoing deformation
Start and End Dates: 01/6/2009 till 31/05/2012
EU Contribution: 2.863.126 €
Coordinator: Prof Vlasis Mavrantzas, University of Patras, GR, vlasis@chemeng.upatras.gr

Modelling

in MONAMI 233513

Subject of the modelling

Molecular- and nano-magnetism, spintronics and magnonics
Quantum transport through materials at nano-scale
Magnetism

Models used

Microscopic, regimes covering the length scales 0.1 – 1 nm:
Density Functional Theory and quantum chemistry models
Exchange-correlation (XC) energy density functional for excited states and time-dependent phenomena
Dynamical Mean Field theory to study material dependent properties of strongly correlated systems like high temperature superconductors
Classical (atomistic) simulation of physical properties of nanostructured materials, using Molecular Dynamics and atomistic spin-dynamics simulations
Mesoscopic regimes covering the length scales 1-100 nm:
Coarse-grained models with effective soft potentials: stochastic terms for essential motions and large-scale structures
Macroscopic regimes covering the length scales larger than 100 nm: continuous medium description using local mass density and energy density thermodynamical or kinetic modeling

Simulation software and type of numerics used

UppAS: Stochastic differential equation, Fokker-Plank equation
RSPt: Matrix diagonalization and invertion, quantum Monte Carlo simulations
NMTO Wannier-like functions for bonding in intermetallic systems
VASP plane wave pseudopotential treatment, Fourier analysis
DALTON quantum chemical first principle theory

Achievements of the model beyond experiments

Modelling of materials properties allows the search for new materials or to make accurate interpretations of observed materials phenomena. An example can be found for magnetic materials where two properties are most important from an application point of view, namely the size of the magnetic saturation moment at room temperature and a large magnetic hardness (or synonymously, a large magnetic anisotropy energy – MAE). These two properties can be predicted for any material, with an accuracy that is needed to make the search for novel permanent magnetic materials much more efficient. The MONAMI project has also led to a soft-ware which enables simulations of magnetization dynamics, where the dynamical movement can be followed for each atom in the simulation, an ability which goes way beyond experimental possibilities.

Application

Electronic and spintronic devices, sensors
Nuclear Magnetic Response probes of electrons in nanoscale system

Relevant review articles

Review of Modern Physics, 82, 1633 (2010); Nature Commun. 105, 1109 (2010); Analen der Physik 523, (2011); Phys. Rev. Lett. 93 27203 (2004) and Phys. Rev. Lett. 96 037205 (2006) Computational Materials Science 55, 295 (2012)

Summary of the project

The project develops novel techniques and paradigms concerning theoretical modelling of nano-scale advanced materials. An important aspect here is the ability to carry out this development all the way from idea and concept to working computer softwares.

Summary of the modelling

The project is focused on developing an understanding of various properties of nano materials by using computer modelling and simulation tools as applicable in different length scales. Ab-inito electronic structure calculations are used in combination with atomistic spin dynamics or molecular dynamics or methods of many-body physics. Density based multiscale modelling is being developed for the properties of nanostructured materials. Furthermore parallel algorithms and a common language between existing software necessary to understand properties of nano-materials is developed.

The project did a study of V_2O_3 to validate a model that was developed within MONAMI, and is a theoretical technique for calculating the effect of electron-electron correlations. The developed models are an elaboration of existing models to make the theory general to treat complex crystal structures like that of V_2O_3. Non–newtonian dynamics was discovered to be necessary for nano-sized magnetic systems of particular symmetries. This was a discovery and/or a numerical result of a simulation tool which was developed under MONAMI, i.e. the UppASD simulation package for spin-dynamics. The non-Newtonian dynamics represents a temporal evolution of a system of classical objects and is incorporated in UppASD. The tail cancellation of orbitals goes long back to a paper by O.K.Andersen, in the 70'ies. It provided new physical insight in how electrons move around in solids, and how to best describe their quantum mechanical equation of motion. In the model developed in MONAMI, several conceptual steps and mathematical derivations have been made to come to a set of equations which enable a numerical implementation. The model now allows accurate and fast calculations of ground state properties of solids.

To be specific, testing of models have been executed to see which one describes the measurements best: a so called N-th order Muffin-Tin Orbital (NMTO) software, with features like massive down folding, generation of Wannier combined, and dynamical mean field theory (DMFT) for the study of strongly correlated system, has been used to investigate the electronic structure of V_2O_3. Also, the development of a full-potential software with incorporation of DMFT has been completed. These theoretical analysis methods are geared towards calculations of spectral properties, which are important when analysing and interpreting the data now emerging from synchrotron radiation facilities and x-ray free electron lasers.

The software package UppASD for the calculation of spin dynamics is continuously being improved. Simulations of nano-magnetism and the dynamical response of small magnetic clusters have been completed and reveal several unexpected phenomena, suggesting a non-Newtonian dynamics of these nano-magnetic systems.

The development of an overlapping muffin-tin approximation (OMTA) transport code has involved replacing the condition of "tail cancellation" of muffin-tin orbitals (MTOs) with "kink cancellation" in an existing tight-binding MTO (TB-MTO) code so as to make maximum use of all of numerical features such as the extensive use of sparse matrix algorithms. This enables calculations of realistic materials, and coupled with transport theory this enables accurate calculations of transport in nano-systems and devices.

The project has also made contributions to the application of a quantum mechanics - molecular dynamics response approach and made applications for calculations of large solvated systems (including more than 10,000 atoms) on their magnetic properties, EPR, NMR parameters, solvatochromism, and non-linear optical properties, like hyperpolarizability and two-photon absorption. In this methodology, the full quantum mechanical interactions are accounted for in the evaluation of a given property. Underlying structures and trajectories are obtained by molecular dynamics or Car-Parrinello methods. Results on protein environments have been obtained and a new technique for parameterization of the electrostatic and polarization interactions in such environments has been developed.

http://www.iacs.res.in/monami/Home.html

Project Acronym and Number: MONAMI 233513
Project Title: Modeling of Nano-Scaled Advanced Materials Intelligently
Start and End Dates: 01/07/2009 till 30/06/2012
EU Contribution: 930.000 €
Coordinator: Olle Eriksson, Uppsala University, olle.eriksson@physics.uu.se

Modelling

in MORDRED 261868

Subject of the modelling

Nanoelectronic devices, oxide interfaces

Models used

Electronic modeling codes: Density functional theory (DFT), drift diffusion (DD) and non-equilibrium Green's function (NEGF) for electron transport
Atomistic modeling: MD including force fields for dynamic charge transfer,
Statistical meso scale models: Monte Carlo (MC)
Device modelling: compact models for extraction engine

Simulation software and type of numerics used

VASP (DFT), CP2k (DFT)
GARAND (DD, NEGF, MC)
Pysic (Molecular Dynamics)
Mystic and RandomSPICE (for compact modeling)
Numerics: genetic algorithms, Bayesian statistics

Achievements of the model beyond experiments

Predict defect character and density that causes device breakdown in realistic environments and over realistic performance times.
Characterize this for a variety of new, industrially untested materials.
Suggest routes for device design that should eliminate or reduce reliability problems

Application

Manufacturing, nanoelectronic devices, transistor and memory design, semiconductors.

Relevant review articles

Nature Insight: Silicon electronics and beyond, Nature 479, 309 (2011).

Summary of the project

Building upon fundamental analysis of the structure and electronic properties of relevant materials and interfaces at the quantum mechanical level, we will construct mesoscale models to account for defect generation and impact on Complimentary-Metal-Oxide-Semiconductor (CMOS) transistor and circuit performance and yield. The models will provide detailed understanding of the common reliability issues and degradation routes of next generation devices. Results will be supported by comprehensive experimental characterization techniques.

Summary of the modelling

The project is performing calculations and characterisation of oxide/semiconductor interfaces in stacks and films.
First principles (e.g. DFT) calculations are used for calculation of interface electronic structure and the impact of defects.
Semi-empirical MD codes are used for e.g. dynamic charge transfer atomistic simulations, for calculations of the structure of large models of the oxide interface.
Statistical models are used to calculate statistical variability of electrical impact of defects and their behaviour as a function of applied bias and time. These are supported by NEGF and drift diffusion simulations directly modelling current within interfaces. The NEGF formalism provides a powerful conceptual and computational framework for treating quantum transport in nanodevices. It goes beyond the Landauer approach for ballistic, non-interacting electronics to include inelastic scattering and strong correlation effects at an atomistic level.
Compact models are semi-physical/phenomenological models of an active circuit component designed to perform high level circuit simulation. There are several variations of the models generally with over 100 Parameters, often tied to a specific simulation methodology.
This results in a realistic description of interfaces in gate stacks, based on combinations of high-k oxides with III-V (GaAs, InGaAs, InP) and IV semiconductors (Si, SiGe, Ge, graphene) and gate metals (TiN, TaN, Ru).

Schottky barrier performance and defects in new gate stack materials are calculated with these models with the goal of improving the reliability of CMOS devices. The thermodynamic stability of defects in different charge states, gap states, optical, electron spin resonance and vibrational properties are calculated. The empirical defect potentials have been optimised using the output of DFT calculations (energy levels, adiabatic potentials, metastable states, vibrational properties). The main defects are associated with oxygen deficiency, interdiffusion of cations, hydrogen and dopants.
The calculated properties of grain boundaries in polycrystalline films, which serve as sinks for vacancies and impurities are used to calculate stress-induced leakage current breakdown mechanisms. Also the dynamic behaviour of the defects and impurities creation and annealing has been studied, in particular the most common defects as oxygen vacancies in their various charge states, dangling bonds at the interface, hydrogen bridges, K centres, etc.
Models and corresponding drift diffusion (DD), monte carlo (MC) and non-equilibrium Green's function (NEGF) simulation tools have been developed that can describe the statistical impact of bias temperature instabilities and hot carriers on the electrical characteristics of CMOS transistors. The simulations are 'frozen' in time. At a particular stage of the degradation process the areal density of defect states and trapped charges is transformed in random defect states and trapped charge distribution that will be introduced in DD, MC and NEGF simulation tools in addition to the initial variability sources. Methods to capture the impact of local defect generation in the gate dielectric on the statistical variation of the gate leakage current have also been developed.

https://webhotel2.tut.fi/fys/mordred

Project Acronym and Number: MORDRED 261868
Project Title: Modelling of the reliability and degradation of next generation nanoelectronic devices
Start and End Dates: 01/04/2011 till 31/03/2015
EU Contribution: 3.624.853 €
Coordinator: Adam S. Foster, Tampere University of Technology, adam.foster@tut.fi

Modelling

in MULTIHY 263335

Subject of the modelling

Microstructure and mechanical properties of materials under the effect of hydrogen embrittlement.

Models used

First-principles DFT calculations for calculations of the energetics of hydrogen in bulk phases and around point defects
Semi empirical Tight binding (TB) and bond order potential (BOP) models for hydrogen interactions with extended defects
Mesoscale Monte Carlo simulations for hydrogen diffusion as function of defect distribution
finite element models of hydrogen diffusion at the continuum, specimen and component levels

Simulation software and type of numerics used

DFT (self-developed codes employing mixed-basis pseudopotential approach, VASP)
TB and BOP codes (self-developed), EAM-Potentials (LAMMPS)
Kinetic Monte Carlo (self-developed codes)
Continuum mechanics (Abaqus, Comsol, Marc, self-developed codes)

Achievements of the model beyond experiments

Optimisation of the pulse-plating process used in the fabrication of the combustion chamber of the Ariane satellite delivery vehicle
Mechanistic understanding of the susceptibility of advanced high strength steels to HE by absorbed H
Prediction of the influence of H on the fatigue lifetime of wind turbine bearings.

Application

Materials for manufacturing, wind turbine, automobile industry, plates for rocket combustion chambers

Relevant review articles

S.M. Myers, M.I. Baskes, H.K. Birnbaum, J.W. Corbett, G.G. DeLeo, S.K. Estreicher, E.E. Haller, P. Jena, N.M. Johnson, R. Kirchheim, S.J. Pearton, M.J. Stavola, *Rev. Mod. Phys.*, 64 (1992) pp559-617

A. Pundt, R. Kirchheim, *Annu. Rev. Mater. Res.*, 36 (2006) pp555-608

I.M. Robertson, H.K. Birnbaum, P. Sofronis, in *Dislocation in Solids*, J.P. Hirth, L. Kubin (Eds.), Vol. 15 (2009) ch91

Summary of project

The aim of the project is to develop a modelling framework to predict the susceptibility of materials and components to hydrogen embrittlement (HE) under conditions representative of those actually occurring in industry. The primary goal is the description of H transport in modern advanced materials with complex microstructures, through development of a multiscale modelling framework. This would provide the basis for an engineer-oriented software tool for the evaluation of the hydrogen embrittlement susceptibility of materials and components based on real microstructural information and environmental conditions occurring in the aerospace, automobile and wind energy industries.

Summary of the modelling

The key aspect of this project is the incorporation of atomistically-derived diffusion barriers for critical H trapping sites into continuum and component level models, and their application to real industrial problems involving HE.

The project is applying density functional theory (DFT) to the evaluation of energy barriers and binding energies of H in normal interstitial sites and around point defects, with consideration given to quantum-mechanical effects. We have also developed semi-empirical tight-binding models and are employing classical potentials for the evaluation of H trapping at extended crystal defects such as grain boundaries and dislocations.

The atomistically-derived results will be used in mesoscale kinetic Monte Carlo (KMC) simulations to evaluate the effective H diffusivities under different strain conditions and trap densities. The ultimate aim of the atomistic-KMC calculations is to develop a database of H diffusivities as a function of defect distribution, stress/strain and temperature. This database would serve as the input for macroscopic (e.g. finite element) models of H diffusion, that could be applied to full components. The models will be applied at the continuum, specimen and component scales using boundary conditions furnished by data collected in-service and from experimental measurements.

The macroscopic models will be based on novel set of constitutive equations for H diffusion capable of exploiting the information being derived from the atomistic calculations. The equations are more generalised than those commonly used in the literature, enabling the description of hydrogen diffusion under a broader range of conditions (e.g. temperature variations, trap occupancies) as before. The equations are being implemented on a number of platforms, including as bespoke codes and as subroutines in commercial FE packages, e.g. ABAQUS. Possibilities for the licensing or commercialisation of these codes will be evaluated during the course of the project.

The modelling will be validated at all levels using advanced experimental techniques (in situ hydrogen permeation tests, thermal desorption spectroscopy, fractography).

The effectiveness of the proposed simulation framework will be demonstrated by investigating the role of microstructure in three contrasting industrial problems, which have been specified by companies involved in the development and application of advanced materials.

http://www.multihy.eu

Project Acronym and Number: MULTIHY 263335
Project Title: Multiscale Modelling of Hydrogen Embrittlement
Start and End Dates: 01/05/2011 till 30/04/2015
EU Contribution: 3.390.722 €
Coordinator: Nicholas Winzer, FhG, DE; nicholas.winzer@iwm.fraunhofer.de

Modelling

in MUST 214261

Subject of the modelling
Inhibitor release, self-healing mechanisms and nanocontainers, formation of containers with membrane emulsification, multifunctional coatings

Models used
Classical Molecular Dynamics
Quantum chemistry electronic model
Multi-phase diffusion equations for water, ions, corrosion products and inhibitor particles in a multilayer anticorrosive film
Dissipative Particle Dynamics (DPD) of the inhibitor/healing agent release under mechanical impact.
Hydrodynamic model of droplet formation in the membrane emulsification process – nonlinear analytical model of formation of containers by membrane emulsification

Simulation software and type of numerics used
Finite Elements and Finite Differences simulation of diffusion
Monte Carlo simulations – lattice gas algorithm
Software for MD calculations, force field Amber 99 – Hyperchem v.8.0, Crystal Maker
Gaussian 03
Mathcad 14.0

Achievements of the model beyond experiments
The model can be used do give recommendation concerning optimal composition and structure of the coating to delay corrosion of metallic and polymeric substrates and structures, thus reducing development costs.
The model predicts service-life time via the probability of the scratch healing or inhibition based on the physico-chemical properties of the materials and realistic scratch geometries.

Application
Coating and surface treatment of metallic and polymeric substrates and structures

Relevant review articles:

Z. Tabor, et.al. .Water Diffusion In Polymer Coatings Containing Water-Trapping Particles, Part 1. Finite Difference - Based Simulations, Progress in Organic Coatings. 75 (2012) 200– 206.

Małgorzata Krzak et. al. . Water diffusion in the polymer coatings containing water-trapping particles, Part 2. Experimental verification of the mathematical model, Progress in Organic Coatings, 75 (2012) 207–214.

N. Filipovic A. Jovanovic et. al. . Modelling of self-healing materials using discrete and continuum methods, Surface Coatings Int., 95 2012 74-79.

Summary of the project

The project MUST developed new active multi-level protective self-healing coatings and adhesives for future vehicle materials that improve the long-term performance of metallic and polymeric substrates and structures. These materials are based on "smart" release nanocontainers incorporated into the polymer matrix of current commercial products.

A nanocontainer (or nanoreservoir) is a nanosized volume filled with an active substance confined in a porous core and/or a shell which prevents direct contact of the active agent with the adjacent environment. The purpose of nanocontainers is to release the inhibitor before corrosion has happened (e.g. in case of presence of aggressive environment) or just after the corrosion has started.

The role of traps is to delay corrosion agents reaching the protected surface.

Summary of the modelling

Two basic mechanisms of corrosion have been modelled. First, the diffusion of corrosive species (e.g. water, chloride ions) through the intact coatings containing traps and inhibitor nanoreservoirs has been modelled by diffusion equations. Second, the release of inhibitor/healing agent upon the mechanical impact during formation of mechanical defects is modelled with the analytical model (geometry), DPD and finite elements and finite differences simulations. Computational algorithms based on Monte-Carlo method for the simulation of the release of healing agent from the microcontainers and its propagation (lattice gas model) during self-healing action has been developed.

The simulation and modelling of the active feedback and self-healing processes have been based on the experimental results obtained on nanoreservoirs and the nanocontainer-containing coatings. This has been used to understand the conditions of effective self-healing (self-healing rate higher than corrosion rate), to feedback to the experimental investigations and to develop new nanocontainers. The output of the modelling can be used to determine the probability of successful healing, i.e. for evaluation of technical risks of application of multilevel protective coating.

Numerical approach for simulation of the layer-by-layer encapsulation process has been developed using combination of QM and MD calculations. Surfactants and polyelectrolytes in solution, their interactions, adsorption at interface and formation of the polyelectrolyte membrane has been simulated according to the following steps:

- Quantum molecular computations for single surfactant molecules and polyelectrolyte monomers for determination of partial atomic charges and electric dipoles.
- Molecular dynamics simulations of polyelectrolyte chains to determine their average conformations, chain stiffness and degree of counterion condensation using AMBER99 force field with corrected van Waals interaction parameters for polyelectrolites in the aqueous medium.
- Molecular dynamics simulation of formation of surfactant-polyelectrolyte complexes and adsorption of single polyelectrolyte chains.
- Molecular dynamics simulation of formation of polyelectrolyte multilayer.

The mean porosity of the polyelectrolyte multilayer membrane was determined taking into account the sum of the solvent accessible volumes of polyelectrolyte chains.

A phenomenological model of formation of liquid emulsion cores by membrane emulsification has been developed. It is based on the balance of hydrodynamic, capillary and buoyancy forces, taking into account the hydrodynamic instability at the formation of droplet at the mouth of the membrane pore. Key parameters for the model have been identified, estimated and verified by measuring the interfacial tension in the system pertinent for emulsification.

Finite differences algorithm for the modelling of the release of corrosion inhibitor based on the solution of the multiphase diffusion equation (in spherical geometry) was developed and applied to the release of 2-mercaptobenzothiazole from the emulsion based nanocapsules.

www.must-eu.com

Project Acronym and Number: MUST 214261
Project Title: Multi-level protection of materials for vehicles by "smart" nanocontainers
Start and End Dates: 01/06/2008 till 31/05/2012
EU Contribution: 7.143.481 €
Coordinator: Theo Hack EADS DEUTSCHLAND GMBH theo.hack@eads.net

Modelling

in NAMASTE 214499

Subject of the modelling

Magnetic and magnetotransport properties of magnetic materials (diluted magnetic semiconductors and transition metal ferromagnets) manipulated by electric fields and strain.

Models used

Band structure calculations, macromagnetic, and elastic theory simulations: model for spin-orbit coupling effects in ferromagnetic metal nanostructures on an atomic level
Ab-initio density functional theory band structure calculations, micromagnetic model for magnetisation, magneto-crystalline anisotropies, damping based on the band structures from the ab-initio, tight-binding, and k•p kinetic-exchange effective Hamiltonian models
Macromagnetic Landau-Lifshitz models
Models of electrostatics, strain and piezoelectric effects
Model for magneto-transport in nano-devices

Simulation software and type of numerics used

Revised k-space integration schemes
Landauer-Buttiker approach for the strongly SO-coupled transition metal systems and for the diluted magnetic semiconductors.
Prague Library of codes suitable for solving these numerical problems

Achievements of the model beyond experiments

Reproduction of the valence band nature of Fermi level states the archetypical ferromagnetic semiconductor (Ga,Mn)As.
Prediction and explanation of the observed magnetic and magneto-transport properties in ferromagnetic semiconductors
Understanding of the observed spin-torque effects which lead to the discovery of new ferromagnetic resonance (FMR) effects.
Based on the developed capabilities to model spin-orbit in metals, it was shown that appropriate antiferromagnetic materials could be employed as active layers in spintronic devices (GMR, etc), thus opening up the possibility of the new field of antiferromagnetic spintronics.

Application

Spintronic and magneto-electronic devices using control and manipulation of the nanoscale magnetic properties through the application of local strain or electric fields.
Antiferromagnetic materials for spintronics
Single ElectronTransistors and Fast Precessional Switching Devices

Relevant review articles

"Spin-orbit coupling induced anisotropy effects in bimetallic antiferromagnets: A route towards antiferromagnetic spintronics", Shick A. B et al., PhysRevB. 81 212409 (2010)
"Magnetocrystalline anisotropies in (Ga,Mn)As: Systematic theoretical study and comparison with experiment", Phys Rev. B 80, 155203 (2009)
"Semiclassical framework for the calculation of transport anisotropies", K. Výborný et al, Phys. Rev. B, 79, 045427 (2009)
"Microscopic mechanism of the noncrystalline anisotropic magnetoresistance in (Ga,Mn)As" K. Výborný et al., 80, 165204 (2009)

Summary of the project

The NAMASTE project aimed to control and manipulate the nanoscale properties of magnetic materials with strong spin-orbit coupling by local strain and electric fields. This should make possible new types of magneto-electronic and spintronic devices. The project explored two parallel complementary strands based on ferromagnetic semiconductors and ferromagnetic metal materials.

Summary of the modelling

The project made detailed microscopic theoretical descriptions of the interrelated structural, magnetic, and electrical properties and their dependencies on a large number of degrees of freedom ranging from the choice of semiconductor host and doping densities to the geometry and arrangement of the nanostructures and spintronic nanodevices.

The spin-orbit band structure was calculated by
a) ab-initio density functional theory
b) multi-orbital microscopic tight-binding theory
c) k•p kinetic-exchange effective Hamiltonian models

Spin-orbit (SO) interaction is at the heart of the materials physics involved and the majority of physical quantities relevant to the experimental work can be derived directly from the SO-coupled band structure of the considered systems. The relevant microscopic micromagnetic parameters include the magnetisation, relativistic magneto-crystalline anisotropy constants, Gilbert damping coefficient, and extraordinary MR coefficients. These have been calculated for metals (ferromagnetic and antiferromagnetic metal alloys), diluted magnetic semiconductors and metal/semiconductor hybrid structures.

Magneto-crystalline anisotropies, e.g., reflect the dependence of the system total energy on magnetization orientation and are sensitive to changes in electron concentration (charge accumulation/depletion in conventional field effect transistor structures) or lattice strains (electrical voltage on piezoelectric transducers). Magneto-crystalline anisotropy then represents the key microscopic input parameter for the micromagnetic Landau-Lifshitz simulations to be employed to describe the magnetization dynamics experiments explored within the project.

Another quantity that can be directly derived from the SO-coupled band structure is the dependence of the position of the chemical potential, at a fixed electron density, on the orientation of the magnetization. The chemical potential anisotropy influences the magnetization reorientation induced Coulomb blockade oscillations, a property exploited in a ferromagnetic Single Electron Transistor. Quantitative modelling of the transport anisotropies in tunnelling or ohmic regime employed the Boltzmann or Kubo transport theories for uniform systems, whereas Landauer-Buttiker and Green's function formalisms were employed for spatially non-uniform nanogeometries and non-equilibrium conditions.

Finally, the magnetic and magneto-transport properties of ferromagnetic semiconductors nanostructures were successfully modelled by combining macroscopic elastic theory and the microscopic relativistic band structure modelling.

http://namaste-project.net/

Project Acronym and Number: NAMASTE 214499
Project Title: Nanostructured Magnetic Materials for nano-spintronics
Start and End Dates: 1/9/2008 till 31/8/2011
EU Contribution: 2.299.963 €
Coordinator: Bryan Gallagher, University of Nottingham, UK, bryan.gallagher@nottingham.ac.uk

Modelling

in NanoInterface 214371

Subject of the modelling
Metal-oxide-polymer adhesion and interface fracture

Models used
Atomistic simulations (quantum mechanics, molecular dynamics and coarse-grained molecular dynamics)
Mesoscale models to describe the competition between cohesive and adhesive failure
Macroscale models to describe the delamination behavior, particle-based mesoscale simulations

Simulation software and type of numerics used
Cross-linking algorithms for epoxy moulding
Materials Studio incorporating Mesocite and COMPASS & EAM for atomistic modelling
LAMMPS for epoxy moulding compounds
Implicit finite local arc-length methodes element

Achievements of the model beyond experiments
A set of design and reliability guidelines for microelectronic packages with respect to delamination risk has been elaborated, which can only be generated in a systematic way by accurate models.
A better, quantitative understanding of adhesion mechanisms at the very small to macroscopic scale and of the effect of surface roughening on adhesion properties has been provided. This was only possible via meso-scale semi-analytical and numerical fracture mechanics models.

Application
Prevention of delamination phenomena in microelectronic packages.

Relevant review articles
Chen J, Bull SJ (2011) Approaches to investigate delamination and interfacial toughness in coated systems: an overview. J.Phys.D: Appl. Phys. 44: 034001.
DeVries KL, Adams DO (2002) Mechanical testing of adhesive joints. In D.A. Dillard, A.V. Pocius (Eds.) The Mechanics of Adhesion, Elsevier.
Hutchinson J, Suo Z (1992) Mixed mode cracking in layered materials. Advances in Applied Mechanics 29: 63–191.
Litteken CS, Dauskardt RH (2003) Adhesion of polymer thin-films and patterned lines. International Journal of Fracture 119/120: 475-485

Summary of the project

In the NanoInterface project a multi-scale modeling approach (atomic, mesoscopic, microscopic, and macroscopic scale) has been applied to describe the failure behaviour of metal-oxide-polymer materials systems. In addition, micro- and nano-scale characterization techniques have been developed and applied. The project focused on the simple and complex carrier systems, defined and processed by industrial partners.

Summary of the modelling

Large scale molecular statics and dynamics simulations were conducted on Cu-Cu tilt grain boundary interface, results of which are used as input to develop interfacial constitutive laws at larger scale. Such models are paramount in developing predictive capabilities related to reliability and failure of microelectronic components. Molecular simulations were conducted on two Cu-Cu tilt grain boundary structures using EAM potential and open source LAMMPS MD simulation code. After obtaining relaxed equilibrium structure (using the coincident-site lattice theory to get the GB interface and conjugate gradient algorithm for energy minimization), it is subjected to Nose-Hoover NPT molecular dynamics with modified Hoover equation of motion under constant strain rate loading. An intergranular crack is introduced and local traction and crack opening displacement data is extracted from the simulation results. To bridge length scales between atomistics and continuum, the data obtained from MD simulations is re-casted within the framework of continuum cohesive zone model (CZM) to quantify the cohesive zone law.

To take into account the influence of roughness on adhesion properties, semi-analytical models at the micro-scale on Cu/Polymer interface are also developed to establish cohesive/adhesive interfacial delamination criteria under external loading. Atomistic simulations on the epoxy resin were conducted to compute its material properties, and interfacial interaction energy on its interfaces with copper and cuprous oxide. A crosslinking procedure consisting of cyclic molecular dynamics simulation/energy minimization and covalent bond creation between reactive sites based on close contact calculation is developed to simulate polymer network formation of the epoxy resin. The cross-linked structure was then fully relaxed to achieve geometry optimization and equilibrated to get rid of artifacts introduced during crosslinking simulation. Subsequent molecular dynamics/molecular statics simulation predicts well material properties, including densities, glass transition temperature, volumetric coefficient of thermal expansion and isotropic mechanical properties, indicating the validity of the adopted polymer network formation methodology. Using the same crosslinking approach, models for interfaces between a 2D polymer network and copper as well as cuprous oxide were constructed and subjected to energy minimization. The interfacial interaction energy for both systems was extracted by the energy difference between the total energy of the entire interface system and the sum of energies of individual components. The system was also subjected to external tensile loading and results related to the interfacial debonding strength are also reported. Interfacial excess energy computation methodology and results for Cu-Cu and Cu-Cu2O interfaces are also presented. Appropriate interatomic potential (IP) formalism is very important to conduct any molecular simulations, as it should be able to capture the correct physics at those loading and environmental conditions. The project also details the IP development framework and results for copper oxide system which is of paramount importance in addressing the failure behavior of the copper/polymer interface which encompasses a thin layer of copper oxide (both, CuO and Cu2O) and invariably influences its failure characteristics.

www.nanointerface.eu

Project Acronym and Number: NanoInterface 214371
Project Title: Knowledge-based multi-scale modelling of metal-oxide-polymer interface behaviour for micro- and nano electronics
Start and End Dates: 01/09/2009 till 31/08/2011
EU Contribution : 3.300.000 €
Coordinator: Dr. Olaf van der Sluis, Philips Applied Technologies, olaf.van.der.sluis@philips.com

Modelling

in NANOMAGMA 214107

Subject of the modelling

Magneto-plasmonic nanostructures

Models used

Maxwell equations in dipole approximation (coupled)

Simulation software and type of numerics used

Generalized Scattering Matrix Methods to solve Maxwell's equations in presence of magneto-optical effects. In various situations it involves a nonlinear eigenvalue problem that, in this case, has been solved by a linearization procedure. The linearization involves an increase in the dimension of the problem. A direct solution would be convenient.
Finite Difference Time Domain solvers, it would be desirable to extend this technology to cope with non-diagonal dielectric tensors for dispersive materials.

Achievements of the model beyond experiments

The model predicted that the optical and magneto-optical response of complex structures where metals and magneto-optical materials are simultaneously present is proportional to the electromagnetic field in the magnetic material. This guided the design and now the whole structure is grown to try to maximize the field in that material.

Application

Non reciprocal devices (Information Technologies devices), Magneto-optical Surface Plasmon Resonance Sensors.

Summary of the project

The goal of this project was the study development and application of a novel concept of nanostructured materials formed by the combination of components with plasmonic and magneto-optic (MO) activity, in order to produce “magneto-plasmonic” nanomaterials tailored on the nanoscale. Both bottom-up and top-down approaches were applied to obtain the desired magneto-plasmonic materials. The goal was to develop films, nanoparticles and core-shell structures. Also proof of concept for applications based on magneto-plasmonic activity is provided including identification of applications for microelectronics and information technology. Testing for specific applications in the field of chemical sensors and biosensors has taken place.

Summary of the modelling

The project modelled the optical response of MO-plasmonic nanostructures using two different approaches: analytical modelling (including the use of approximate methods) and quantitative numerical simulation. Both approaches are complementary and necessary in order to reach the main objectives.
Using the procedure described above the project explored the mechanisms that would allow:
i) Investigate the correlation between the optical, magnetic, magneto-optical and magneto-plasmonic properties.
ii) Controlling the plasmon (either surface or localized) using an external magnetic field.
iii) Analyzing the interplay between plasmon excitation and MO response.
iv) Amplifying the MO response from local field enhancements

The project performed:
• Numerical calculation of the MO response of continuous trilayered structures solving the Maxwell equations using transfer and scattering matrix techniques (layer thickness optimization for maximum sensor signal in Au/Fe/Au structures).
• Analysis of magneto-plasmonic periodic arrays of small particles coupled to a multilayer structure described by the Maxwell equations in the dipole approximation.
• Analysis of the MO properties of a random dispersion of magnetic nanoparticles (using the coupled dipole method).
• Comparison between SNOM measurements and calculations of near-field signals on magneto-plasmonic structures.
• Numerical study of field enhancements on magneto-plasmonic structures for molecular sensing.
• Quantitative study of single-molecule fluorescence control by magneto-plasmonic structured substrates or nanoparticles.

http://www.phantomsnet.net/Nanomagma/indexMagma.php?project=5&f=1

Project Acronym and Number: NANOMAGMA 214107
Project Title: NANOstructured active MAGneto-plasmonic MAterials
Start and End Dates: 01/11/2008 till 31/10/2011
EU Contribution: 2.963.156 €
Coordinator: Antonio Garcia-Martin, Instituto de Microelectronica de Madrid, Consejo Superior de Investigaciones Cientificas, Madrid, ES, e-mail: a.garcia.martin@csic.es

Modelling

in NANOMODEL 211778

Subject of the modelling
Mechanical, thermochemical and flow behaviour of nano-filled polymeric materials

Models used
Molecular Dynamics (MD) techniques for nanomechanics
Micromechanics model
Mesoscale methods (CG coarse grained MD) for what property/process in nanostructure and nanomechanics
Dissipative Particle Dynamics (DPD) for nanostructures
Field Theory inspired Monte Carlo (Fti-MC) for nanostructures

Simulation software and type of numerics used
FEM for micromechanics
Coupling schemes between Molecular Dynamics and Continuum Mechanics, based on modified Arlequin algorithm
Integrated software product Culgi to model and visualize nanocomposites

Achievements of the model beyond experiments
The role of the interphase (structure and dynamics) is difficult to investigate experimentally. Only modelling can give access to the very structure of matrix, nanoparticles and their interphases. Modelling revealed details how the interface is influenced by the chemistry.

Application
Reinforcement of polymeric material
Surface modifiers ensuring stable particle dispersion under melt mixing conditions

Relevant review articles
Attinger, S., Koumoutsakos, P. (Eds.), Multiscale Modelling and Simulation, Lecture Notes in Computational Science and Engineering Vol. 39 (Springer, Heidelberg, 2004)

Summary of the project
The project targets the reinforcement of polymers via the decrease of viscosity through admixture of nanoparticles. The project has studied the detailed structure of matrix, nanoparticles and interface region. By detailed comparisons of computed structures and experimental ones, new composites were explored.

Summary of the modelling
The project dealt with the coupling of continuum mechanics CM (please explain which mecahnics process and which constitutive equations you used; Finite Element (FE) method is only the solver , not the physics) with particle based Molecular Dynamics (MD) methods.
The CM and MD part have been adapted as follows: in the MD part, the necessary number of degrees of freedom has been reduced by coarse graining, i.e. groups of atoms are considered as single super atoms. Furthermore, the periodic boundary conditions (PBC), which avoid surface effects in the MD simulation box, have been replaced by stochastic boundary conditions (SBC), combined with a DPD thermostat. Using a certain probability function in the boundary domain, a part of the super atoms in that region is tethered via a harmonic interaction potential to so-called anchor points. These additional artificial particles transfer information (forces and positions) from the MD region to the FE domain and vice versa. The main advantage of this approach is the spatial fixing of the anchor points during the MD run, thus there is no dynamic coupling to FE required. The rigid frame of anchor points enclosing the MD domain is coupled to the FE domain by using the Arlequin method which is based on an energy blending of the different domains.

A coupling algorithm between MD (Molecular Dynamics) and CM allows for the computation of forces externally exerted on a nanocomposite. The multiscale approach to study the structure and dynamics of e.g. silica-polystyrene nanocomposite systems consisted of four levels of description: an atomistic one, several coarse grained ones where each “superatom” or bead represents e.g. a monomeric unit or a meso or racemo diad of styrene monomers, parametrized using Iterative Boltzmann Inversion (Coarse Grained Monte Carlo, CG-MC), or DPD, and a third one describing the system at a length scale comparable to that of the Kuhn length, by exploiting the polymer mean field approximation (Field Theory – inspired Monte Carlo, FT-i MC), and a micromechanical approach based on mesoscale morphologies. The first two levels of modelling are closely connected, via forward and reverse mapping schemes. Initial configurations have been subjected to CG-MC simulations, where polymeric chains were e.g. treated as chains of diads and nanoparticles as solid spherical Hamaker interaction sites. Based on atomistic molecular dynamics trajectories of the equilibrated structures, local packing and dynamics were addressed by calculating pair distribution functions, bond orientational autocorrelation functions and H-NMR spectra. The third level of modeling (FT-i MC) has enabled simulations of micrometer-sized domains of the nanocomposite system, wherein the nanofillers are represented as solid spheres (interacting via Hamaker integrated potentials) and the polymer chains as freely jointed sequences of Kuhn segments.
The protocols developed for the model Polystyrene systems were applied to other systems identified by the consortium as interesting for applications, such as PMMA, Nylon 66, and PBT SiO2 based nanocomposites. A pseudo core-shell model to account for interface phenomena in the multiscale procedure was developed and tested on unmodified spherical and cylindrical nanoparticles based nanocomposites.

https://nanomodel.eu/

Project Acronym and Number: NANOMODEL 211778
Project Title: Multi-Scale Modeling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance
Start and End Dates: 01/11/2008 till 30/11/ 2011
EU Contribution: 3.481.149 €
Coordinator: Horst Weiss, BASF SE, Horst.weiss@basf.com

Modelling

in Next-Gen-Cat 280890

Subject of the modelling

Catalysts consisting of transition element metal nano-particles without Platinum Group Metals (PGM)

Models used

Electronic modelling: ab initio quantum mechanical model and DFT for surface energies and activation energies of the catalytic nanoparticles
Continuum modelling: simulation of the species concentration in the gas and the kinetics of the reactions

Simulation software and type of numerics used

Home made codes (on Matlab etc) and a process simulator like ASPEN and CFD simulator will be used. Additionally commercial/open source codes include Cantera, CHEMKIN, DETCHEM, Comsol
Commercial and/or academic programs Gaussian 03/ Vasp/ Quantum Expresso/ ADF

Achievements of the model beyond experiments

Improved understanding of catalytic reactivity on non-PGM catalysts

Application

Nanoparticles of transition elements based catalysts for automotive sector

Relevant review articles

L.L. Raja, R.J. Kee, O. Deutschmann, J. Warnatz, L.D. Schmidt, A critical evaluation of Navier–Stokes, boundary-layer, and plug-flow models of the flow and chemistry in a catalytic-combustion monolith, Catalysis Today 59 (2000) 47-60.
Paolo Giannozzi, et al. “QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials” J. Phys. Cond. Matter, 21 (2009) 395502.
H. Santos and M. Costa “Modelling transport phenomena and chemical reactions in automotive three-way catalytic converters” Chemical Engineering Journal 148 (2009) 173–183.

Summary of the project

The main objective of NEXTGENCAT proposal is the development of novel eco-friendly nano-structured automotive catalysts utilizing transition metal nano-particles (Cu, Ni, Co Zn, Fe etc) that can partially or completely replace the PGMs.

Summary of the modelling

The project addressed physicochemical phenomena concerning nanostructured catalysts..
The project will apply existing models and the aim of the modelling activities within the NEXT-GEN-CAT is to check initially the validity of the current available models and /or to adjust their parameters in order to comply with the experimental data obtained either by the literature or by experiments performed by the consortium. After the validation of the models certain runs will be performed in order to predict the behaviour of a catalytic system without the need to perform the experiments. Therefore, only selected catalyst will be evaluated using real feed conditions. The results of the nano-scale modelling will be used later for the process engineering and the optimization of the catalytic performance.

Materials at nanoscale
The surface of the catalysts will be calculated at the atomic level in order to understand the interaction between the gas phase molecule and the catalyst. The stability of all exposed surfaces will be computed from first principles calculations. It will be possible to modify the composition of the surface to determine the most promising catalysts. These studies will the focus on the active phase composed of catalysts. The computed surface energies will be used to build the most probable shape of the nanoparticles.
The chemical properties of the surfaces will be computed using the quantum formalism (Schrödinger Equation). Due to the size of the system model, DFT approach (Kohn- Sham equation) will also be applied.
In a second step, the reaction mechanism will be calculated as well as the activation energies that can be used latter in kinetic models for the process simulation of the catalysis.
The equilibrium shape of crystals can be predicted from the Wulff construction, which in turn is obtained from the surface energies of the most stable surfaces of the material.

Process Simulation
The models to be applied will simulate the performance of the catalytic converters and predict the concentration distribution of the chemical species in the gas and the temperature profile inside the converter as well as the velocity profile. More specific the models will enable the:

- simulation of the species concentration in the gas (near and far from the catalytic surface, along the flow direction), on the surface, and the corresponding temperature, pressure and velocity variation along the converter.
- tuning of a kinetic submodel, including detailed surface chemistry and possibly gas-phase reactions, able to make simulation consistent with experimental data. Initial kinetic parameter will hopefully be provided within the project dedicated to more fundamental approaches (nanoscale modelling).

The equations governing the simulation are the kinetic equations, and the equations produced from the mass balances of the chemical species, the heat balance and the momentum balance will be applied. Furthermore, material, energy and momentum balances, in differential form and at any direction where gradients are expected (along and across the flow) will be considered using ordinary differential equations (ODEs) or partial differential equations (PDEs)

www.nextgencat.eu

Project Acronym and Number: Next-Gen-Cat 280890
Project Title: Development of NEXT GENeration cost efficient automotive CATalysts behaviour for micro- and nano electronics
Start and End Dates: 01/02/2012 till 31/01/2016
EU Contribution: 3.940.000 €
Coordinator: Fotis Katsaros, Demokritos, EL, fkats@chem.demokritos.gr

Modelling

in NIM_NIL 228637

Subject of the modelling
Characterisation of electromagnetic metamaterials

Models
Application
Electromagnetic wave theory for characterisation, Maxwell's equations coupled to constitutive equations for material response; constitutive equations are dispersive models (Drude, Drude-Lorentz) or experimentally obtained material constants; Rigorous Coupled Wave Analysis (RCWA) method is used to calculate transmission and reflection and field distributions inside the metamaterial structures.
Development
Models for losses

Simulation software and type of numerics used
Commercial software, DiffractMOD (RSoft inc.), Reticolo and RCWA solver
Self-written Mathematica and Matlab codes for implementation of Berreman formalism for oblique incidence retrieval and visualization purposes
Finite-difference time-domain method, finite-elements method (COMSOL), finite integration technique (CST Microwave Studio), retrieval procedure based on scattering parameters.
RCWA method solving Maxwell's equations for stratified structures like gratings and metamaterials
Simulated structures are assumed periodic in lateral dimension and the accuracy can arbitrarily be increased by taking a higher number of Fourier harmonics and better discretization

Achievements of the modelling beyond experiments
Negative refractive indices cannot be measured directly but need to be carefully derived from measurements.
Determination that silver is the best conducting material for use in optical metamaterials
Design and optimization of 3D metamaterial structures
Unambiguous demonstration of negative refraction with wedge configuration for designed negative index metamaterial in the visible regime

Application
Optical devices for communications and imaging

Relevant review articles
http://ec.europa.eu/research/industrial_technologies/pdf/metamaterials-brochure_en.pdf
C. M. Soukoulis and M. Wegener, "Past achievements and future challenges in the development of three-dimensional photonic metamaterials," Nature Photon. **5**, 523-530 (2011).
G. W. Hanson, J. Appl. Phys. 103, 064302 (2008).
J.W. Weber et al., Applied Physics Letters 99, 061909 (2011)
Oates et al., Optics Express 20(10) 11166 (2012)

Summary of project

The aim of NIM_NIL is the development of a production process for 3D negative refractive index materials in the visible regime combining UV-based nanoimprint lithography (UV-NIL) on wafer scale using the new material graphene and innovative geometrical designs.
A micro-optical prism will be fabricated to directly verify and demonstrate the negative refractive index.

Summary of the modelling

Electromagnetic characterisation tools are used to interpret the measured reflection and transmission by spectroscopic ellipsometry to determine the region of negative refractive index and its dispersion as a function of wavelength. Dependence on the wave vector is also investigated. During the characterization stage ellipsometry and normal incidence responses of the models were compared with post fabrication measurements to calculate effective parameters of the product. Then necessary feedback was given to the fabrication team for further optimizations.
The optical properties of graphene are not completely characterized experimentally, especially in the infrared and Terahertz frequency regions. Relations between the density of free carriers and the frequency dependent conductivity as a function of the temperature and the Fermi level (which may be influenced by external bias) are established. The relation is based on the Drude model using the Kubo formula. We used these formulas as input to the dielectric functions to fit our infrared ellipsometry measurements. We used the Airy-Fresnel formulas to create a layer model of the substrate and graphene layer, and fit the optical conductivity (dielectric functions) in the range from 600-4000 cm-1. In this way we could estimate the Fermi level shift due to chemical doping from atmospheric exposure.
We also characterized the plasmonic modes of silver fishnet metamaterials fabricated using nanoimprint lithography. Coupling of obliquely incident radiation to surface plasmon polaritons (SPPs) at a metal-dielectric interface is affected when the incident wave vector matches an SPP wave vector. We used the SPP formulas coupled to the grating formulas to show the angular dependence of the SPP modes in spectroscopic ellipsometry data.

Full-wave simulations are used for the calculation of scattering parameters of metamaterial structures. The scattering parameters can subsequently be used to determine the effective material constants of the metamaterials. The models were used for the design of the metamaterial samples. Full-wave simulations were performed for metamaterial wedges. This effort used our existing numerical simulation capabilities, but it was scaled up to accommodate the large computational problem involved. Wedges contain many circuits and require resolving the electromagnetic on both the microscopic and macroscopic scales. Possible candidates for optical metamaterials with negative index of refraction were identified. The improved wedge configuration shows unambiguous phenomenon of negative refraction with designed optical metamaterials. Single and multiple functional layer Fishnet metamaterial in IR and visible regions were designed and simulated using ab-initio Maxwell solver (RCWA).
A EM model was developed to describe the dissipative loss in resonant electromagnetic metamaterials. The model takes into account the radiation damping of the resonant currents, which is necessary to model metamaterials made from low-loss conducting materials. This model led to an identification of which conducting materials are useful for metamaterials. Silver was found to be the best conducting material at optical wavelength. Graphene was ruled out.

www.nimnil.org

Project Acronym and Number: NIM_NIL 228637
Project Title: Large Area Fabrication of 3D Negative Index Metamaterials by Nanoimprint Lithography
Start and End Dates: 01/09/2009 till 31/08/2012
EU Contribution: 3.373.100 €
Coordinator: Iris Bergmair, Profactor, DE, iris.bergmair@profactor.at

Modelling

in NPMIMETIC 246351

Subject of the modelling
biomaterials, biomimetic nano-polymer gel, synthetic scaffolds

Models used
Model for hyperviscoelastic behavior in biomaterials
Multibody system dynamics model (MBS) for Intervertebral disc loading conditions incorporating local (biomaterial) physics

Simulation software and type of numerics used
Partial differential equations for finite element methods (model for hyper viscoelastic materials) and multibody system dynamics
Algorithms for image analysis (denoising, segmentation, smoothing, sampling and visualisation)

Achievements of the model beyond experiments
The study of the intervertebral disc (IVD) mechanical behaviour presents a high level of difficulty, due to intrinsic uncertainty on the quantification of real working loads (coupling compression forces, flections and torsion moments). Post-mortem analysis doesn't allow a full understanding of these phenomena, mainly due to the highly hydrated nature and the fact that the osmotic role of nucleus function is not achieved in those conditions. Modelling can overcome these restrictions and predict two fundamental situations:
i)degenerated IVD – stress/strain conditions due to nucleus degeneration (geometry, stress conditions, prediction of overstretched annulus' fibres)
ii) restored IVD – prediction of restoration conditions, annulus rupture state and/or failure risks on the nucleus 'refilling' process, influence of nucleus prosthetic materials characteristics on overall mechanical stability

Application
Biomedical implants for intervertebral discs

Relevant review articles
Cavalcanti, C; Alves, JL, Mechanical behaviour and constitutive modelling of the annulus fibrosus: a literature review, ESB-2012, 18th Congr. European Society of Biomechanics, Lisbon, Portugal, Jul. 2012

Araújo, A; Peixinho, N; Marques Pinho, AC, Stress characterization of intervertebral disc on radial direction: an experimental approach, ESB-2012, 18th Congr. European Society of Biomechanics, Lisbon, Portugal, Jul. 2012

Summary of the project

The NPmimetic project will develop a biomimetic nano-polymer based gel for minimally invasive disc regeneration treatment: Electro-spinning technology will be exploited to design and develop a nano-fiber based, biocompatible, biodegradable, synthetic scaffold that will mimic the mechanical properties of the native nucleus pulposus (NP) for immediate and short term treatment. Anti-inflammatory drugs will be carried by the biodegradable nano-fibers to be gradually released in situ for healing and preventing inflammation.

Summary of the modelling

The models developed are focused on three main objectives:
1. prediction of the mechanical behaviour of an undamaged intervertebral discs, and possible geometrical/mechanical effects of a NP pathology;
2. virtual simulation of the NP regeneration, and assessment to the bio-mimetic gel withstanding loads and behaviour characteristics under working conditions;
3. assistance in the evaluation of eventual different proposals to the therapeutic modalities and/or techniques of regeneration.

Intervertebral disc geometry definition involved the development of an automated image-based procedure, capable of making a sound identification of soft tissues and substrate bone (i.e., capable of distinguishing between muscle and ligaments, tendons and bones, cortical and trabecular bone, fibrous and pulpous regions, etc.), extracted from 2D high resolution MRI or other available technique images.A subroutine was created to built up geometrically consistent boundaries/regions, through analysis, parameterization and high-degree regression of 2D topographic curves, in order to produce suitable 3D meshed ‘solid’ entities.

A hyper-viscoelastic model for bulk material, with an almost incompressible assumption was used in a non-linear finite elements model (FEM) approach to mimic Nucleus pulposus (NP) behaviour within the intervertebral discs.

Intervertebral disc loading conditions were simulated with a multibody system (MBS). This can, with a much lighter computational effort than FEM, simulate the dynamic behaviour of the mechanical phenomena inside the intervertebral discs, either under endogenous or exogenous actuations, and a detailed analyse of the localized deformation on intervertebral disc’s soft tissues can be achieved.

Combining all these aspects, a hybrid model can be developed, using the multi body system tool to predict the motion of the segment and the FEM tool to detailed analyse the localized deformation on IVD’s soft tissues. The kinematics, stress distribution and its effects can be analyzed simultaneously, allowing a more precise definition of the loading state of the different parts in different situations, as well as the prediction of the overall behaviour of the set under ‘real’ use.

Project Acronym and Number: MODIFY 228320
Project Title: Biomimetic nano-fiber-based nucleus pulposus regeneration for the treatment of degenerative disc disease
Start and End Dates: 01/02/2011 till 31/01/2015
EU Contribution: 3.985.587 €
Coordinator: Marco N Helder, Vrije Universiteit medical center, Amsterdam, NL m.helder@vumc.nl

Modelling

in ONE-P 212311

Subject of the modelling
Electronic processes occurring in organic-based devices (charge transport, light conversion into current, charge injection) and their dependence on system morphology.

Models used
Ab initio or semi-empirical Hartree-Fock methods, DFT methods, Molecular Dynamics, Molecular Mechanics, Quasi-Harmonic Lattice Dynamics, Kinetic Monte Carlo algorithms.

Simulation software and type of numerics used
Gaussian, Ampac, ADF, SIESTA, Gromacs, Materials Studio, Tinker, NAMD

Achievements of the model beyond experiments
Material design targeted to the optimization of physical properties and to yield devices with enhanced efficiencies. Modelling allowed the fast screening of candidate molecules for electron transport in devices, IR emitters and lasing applications. It predicted organic semiconductor crystal structures and explained the influence of lattice mismatches at the interface between two crystalline organic semi-conductors on the interfacial electronic properties; and predicted its implications for charge separation in organic solar cells.

Application
OLEDs, field-effect transistors, sensors and storage devices, solar cells

Relevant review articles
"An Atomistic Description of Polymer Dielectrics/Pentacene Interfaces: Influence of Electrostatic Interactions on Charge Mobility Values". N.G. Martinelli, M. Savini, L. Muccioli, Y. Olivier, F. Castet, C. Zannoni, D. Beljonne, and J. Cornil. Advanced Functional Materials 19 (2009) 3254-3261.

"Control of the Mutual Disposition of Cyclometalated Ligands in Cationic Ir(III) Complexes: Synthesis, Spectroscopy, and Device Efficiency of the Different Isomers". J.M. Fernandez-Hernandez, C.H. Yang, J. Beltran, V. Lemaur, F. Polo, R. Frölich, J. Cornil, and L. De Cola. Journal of the American Chemical Society 133 (2011) 10543-10558.

Photoinduced Work Function Changes by Isomerization of a Densely Packed Azobenzene-Based SAM on Au: A Joint Experimental and Theoretical Study". N. Crivillers, A. Liscio, F. Di Stasio, C. Van Dyck, S. Osella, D. Cornil, S. Mian, G.M. Lazzerini, O. Fenwick, E. Orgiu, F. Reinders, S. Braun, M. Fahlman, M. Mayor, J. Cornil, V. Palermo, F. Cacialli, and P. Samori. Physical Chemistry Chemical Physics 13 (2011) 14302-14310.

Summary of the project

ONE-P developed new functional organic materials for organic electronics and photonics and some applications such as organic light-emitting diodes, photovoltaics and active matrices. These materials provided enhanced properties in electron transport, conversion of photons into electrons and/or conversion of electrons into photons and can be printed in a continuous process.

Summary of the modelling

ONE-P applied modelling approaches in order to investigate electronic and structural properties of the next generation of organic conjugated compounds for applications in organic electronics. The project achieved

- The elaboration of design rules for improving the charge transport properties of n-type as well as ambipolar organic semiconductors by combining Molecular Dynamics simulations for the prediction of the bulk organization, quantum-chemical calculations for the evaluation of the molecular parameters defining the rate of charge transfer between molecules and Kinetic Monte Carlo algorithms for the propagation of the charge and the evaluation of the charge carrier mobility.
- The impact of the nature of the insulating layer in field-effect transistors on the electrostatic disorder at the interface between the dielectric layer and the organic semiconducting layer. We have used here a combination of Molecular Dynamics simulations to generate realistic interfaces between the insulating layer and the organic semiconductor at the nanometre scale, quantum-chemistry and Kinetic Monte Carlo approaches to quantify the impact of different dielectrics on the charge carrier mobility.
- The development of a methodology to model the triplet energy transfer at the molecular scale from quantum-chemical calculations to end up with exciton diffusion length using Kinetic Monte Carlo.
- The modelling of the relationship between the structural organization of polymer chains modelled by Molecular Dynamics and the solid-state optical properties described by phenomenological models.
- The modelling of realistic donor-acceptor interfaces (such as polymer-fullerene) using Molecular Dynamics simulations in order to extract by means of quantum-chemical calculations the dipole at the interface between organic layers.
- The rational design of functional molecules for SAMs for application in molecular electronics by means of Non-Equilibrium Green's Function DFT calculations.
- The modelling of the changes in the work function of metal electrodes upon deposition of self-assembled monolayers or organic semiconductors using DFT calculations with Periodic Boundary Conditions (as implemented in SIESTA) to tune the charge or spin injection barriers.

http://www.one-p.eu/public/

Project: 212311 ONE-P
Title: Organic Nanomaterials for Organics and Electronics
Start and End Dates: 01/01/09/2009 till 31/12/2012
EU Contribution: 17.989.000€
Coordinator: Prof. Yves Geerts, ULB, BE, ygeerts@ulb.ac.be

Modelling

in ORAMA 246334

Subject of the modelling

Multifunctional oxides (Active Semiconductor Oxides (ASO))
Passive n-type amorphous Transparent Conducting Oxides (a-TCOs) and p-n type junctions thereof

Models

Electronic model: First principle modelling (DFT) of oxide materials for the electronic structure of oxides
Generalized Boltzmann Transport Equations models for plasma and thin film growth
Computational fluid dynamics for droplet formation

Simulation software and type of numerics used

Own codes: BEM for electric field computation by Poisson's equation
PICMC Parallel Particle-in-Cell Monte-Carlo code including routines for particle motion (DSMC)
BEM for electric field computation by Poisson's equation
RIG-VM for computation of magnetic fields using the Boundary Element Method
CFX Ansys (CFD)
Commercial software: Advanced, Essential Macleod, Code and OptiLayer
Scripting language used for scheduling of parallel simulation tasks, for specialized post-processing and for optimization issues.
Direct Simulation Monte-Carlo (DSMC) techniques.
Optical analysis codes

Achievements of the modelling beyond experiments

Using modelling, we understood the relevance of the grain boundaries for shallow acceptor levels which are the prerequisite for p-doping in ZnO films with substantial resource savings compared with an experimental approach. Similar savings are achieved for the layout of deposition chambers and coating processes. Our modelling allows for an in depth understanding of the plasma parameters and growth conditions particular in PVD processes. The modeling of particle fluxes and energies allows for substantial time savings and deeper understanding compared to experiments.

Application

Electronic devices (automotive),Thin film photovoltaics, Displays, LED and OLED technology

Relevant review articles

B. Szyszka et al., Development of new transparent conductors and device applications utilizing a multidisciplinary approach, Thin Solid Films 518 (2010) 3109
B. Szyszka et al., Recent developments in the field of transparent conductive oxide films for spectral selective coatings, electronics and photovoltaics, Current Applied Physics 2012, in press, doi: 10.1016/j.cap.2012.07.022
W. Körner et al., First-principles density functional study of dopant elements at grain boundaries in ZnO, Phys. Rev. B 81 (2010) 085324
M.Putti, et al., "New Fe-based superconductors: properties relevant for applications" Supercond. Sci. Technol. **23** (2010) 034003
K. Tanabe and H. Hosono "Frontiers of Research on Iron-Based Superconductors toward Their Application" Japanese Journal of Applied Physics **51** (2012) 010005
G. R. Stewart "Superconductivity in iron compounds" Reviews of Modern Physics, **83** (2011) 1589

Summary of project

Orama deals with the development of multifunctional oxide based electronic materials, processable at low temperatures, including flexible substrates. Orama will address the potential of oxides as electronic materials in the automotive industry. It will achieve this by addressing the four key elements being essential for building up the new era of oxide based electronic industry: 1st principle material modelling, synthesis of new materials, development of low temperature and damage free deposition and patterning techniques and novel characterization methods.

Summary of the modelling

The materials modeling in Orama aims at understanding of semiconductor properties for realistic life materials including doping and defect related phenomena. An important issue is the understanding of p-conductivity in doped ZnO films and novel p- and n-type oxide materials. Another important issue is the suppression of plasma damage due to high energetic species impinging on the substrate.
A multiscale model for coating processes is used. To achieve this, we use different approaches to model electronic structure, plasma process and thin film growth phenomena and for continuum modelling of ink-jet processes.

First principle modeling of the electronic structure of oxides

Own code developments or source codes available for academic purposes were utilised to solve the Kohn-Sham equations of density functional theory for the first principle modelling of the electronic structure including defect effects, such as doping and grain boundary related issues.

Plasma and thin film growth related phenomena

For these areas, codes developed earlier were used. Monte-Carlo techniques were used to solve the Boltzmann transport equation for the description of gas flow phenomena by means of Direct Simulation Monte-Carlo (DSMC) techniques. With self-consistent electric field computation that approach is extended to Particle-in-Cell Monte-Carlo Techniques (PIC-MC) for plasma phenomena. The simulation environment is entitled “picmc“. RIG-VM is used for scheduling and parameterization of the parallel computing jobs. Further, it can be used for specialized post-processing and optimization issues. Besides PIC-MC simulation, RIG-VM comprises a module for optical simulation of multilayer stacks.
Computational fluid dynamics (CFD) modelling is used for various tasks in the optimization of Ink-Jet and Sol-Gel processes. Here, we use commercial software, from suppliers such as CFX / Ansys.

Optical analysis

Here, we use also the RIG-VM code to model optical spectra and X-ray reflectometry data besides several commercial products in this field (such as Advanced Fit by Sentech, Essential Macleod, Code or OptiLayer.
An important application is the model based analysis of RF-superimposed DC-sputtering of TCOs serving as front contact for thin films LEDs where intense bombardment reveals plasma damage (due to release of N from the GaN substrates) which increases the operation voltage of the device.

Project Acronym and Number: ORAMA 246334
Project Title: Oxide Materials Towards a Matured Post-silicon Electronics Era
Start and End Dates: 01/10/2010 till 30/09/2014
EU Contribution: 9.742.506 €
Coordinator: Bernd Szyszka FhG, DE, coordination@orama-fp7.eu

Modelling

in OXIDES 228989

Subject of the modelling

Oxide interfaces and nanostructures (structural, electronic and functional properties)

Models used

Electron models:

First-principles description within the Density Functional Theory formalism

Second-principles modeling: Tight-binding Hamiltonians for electrons, Effective Hamiltonians for the lattice-related properties at finite temperatures, Bloch-Boltzmann theory for transport and thermoelectric properties, Brinkman-Dynes-Rowel model for tunnel junctions

Simulation software and type of numerics used

Standard packages for first-principle simulations (SIESTA, ABINIT, CRYSTAL, VASP) and home-made/open-source codes (BoltzTraP) for second-principles simulations

Iterative resolution using either a variational formulation and a minimization method or a diagonalization procedure

Parallelised code

Achievements of modelling beyond experiments

Theoretical predictions to be further validated experimentally:

The unexpected possibility to induce multiferroism in epitaxially strained $CaMnO_3$

The unexpected possibility to achieve exploitable Tunnel Electro-Resistance (TER) in symmetric Ferroelectric Tunnel Junction (FTJ); for memory applications

The prediction of the unexpected appearance of a half-metallic ferromagnetic highly-confined 2-dimensional electron gas (2DEG) in $SrTiO_3/SrRuO_3$ superlattices

The unexpected role of oxygen rotation in shifting by 300 K the ferroelectric phase transition of $PbTiO_3$;

Joined theoretical-experimental breakthroughs

Improper ferroelectricity in oxide superlattices in which modelling identified a new microscopic mechanism (the so-called trilinear coupling of structural instabilites) as observed in parallel experimentally

Exchange bias in $LaNiO_3/LaMnO_3$ superlattices; modelling allowed the proper understanding of the unusual spin order giving rise to the experimental results

Compelling evidence of the intrinsic nature of the 2DEG at polar oxide interfaces; modelling of ideal interfaces was required to unambiguously distinguish between intrinsic and extrinsic effects

Confinement properties of the 2DEG at the $LaAlO_3/SrTiO_3$ interface; modelling provides key information on the electronic band structure, mandatory to interprete measured properties

Application

Nanostructures for electronic and spintronic applications, ferroelectric and multiferroic memories, thermoelectric devices for energy conversion and energy harvesting

Relevant review articles

ABINIT: first-principles approach to material and nanosystem properties X. Gonze et al.Computer Physics Communications 180, 2582 (2009)

Summary of the project

The OxIDes project develops advanced techniques for the atomic scale modelling of the most relevant types of oxide interfaces and uses these tools to design a new generation of layered materials with unique experimentally-confirmed properties.

Summary of the modelling

OxIDes uses a multi-scale approach to address the physics of three types of interfaces: (i) insulating interfaces between insulating oxides, where coupling between lattice modes can lead to unusual phenomena; (ii) conducting interfaces between insulating oxides, where an interfacial 2-dimensional electron gas (2DEG) might exhibit large thermoelectric power; and (iii) interfaces between metallic and insulating oxides, for a deeper understanding of screening.

OxIDes relies at a first level on advanced atomic-scale modelling based on first-principles Density Functional Theory (DFT) techniques where the study of highly-correlated electron sytems and/or specific interfaces (like metal/insulator interfaces) requires going beyond the usual approximations. Significant methodological advances concern the use of pseudo self-interaction correction local density functional method pSIC and B1-WC hybrid functional techniques for these interfaces. The pSIC method removes in complex systems the spurious self-interaction repulsion present in local or semilocal density functionals (LDA, GGA). The B1-WC functional was introduced only recently and implemented in CRYSTAL code during the project. Hybrid functionals are well known but this is a new functional that was adjusted to properly describe at the same time the lattice dynamics and electronic properties of functional ferroelectric and related perovskites. Previous hybrid functionals were not satisfactory for those systems. A variational pSIC extension was developed within Oxides allowing atomic relaxation at the pSIC level. In the VPSIC approach, the atomic forces formulation follows from the usual Hellmann-Feynmann procedure. It is obtained as the LSDA expression augmented by a further additive contribution due to the atomic-site dependence of the SI projectors.
The first-principles techniques have been used to study single- and poly-domain structures of ferroelectric capacitors and various ABO_3/$A'BO_3$ superlattices, the origin and confinement of the 2DEG at the $LaAlO_3$/$SrTiO_3$ interface or in $SrRuO_3$/$SrTiO_3$ superlattices, the magnetic properties of nickelates, etc.

The second-principle modelling includes a tight-binding hamiltonian for electrons to determine the equilibrium distribution of the conduction charge in 2DEG, extended effective Hamiltonians for finite-temperature simulations of ferroelectric-related properties, an approach based on Bloch-Boltzmann theory for the prediction of thermoelectric properties and the Brinkman-Dynes-Rowel model for the determination of electronic transport properties. OxIDes developed a totally new effective Hamiltonian approach, that properly includes all ionic degrees of freedom, for the study of structural phase transitions with temperature, implemented a method including a temperature-dependent relaxation time for the description of the transport properties within the Bloch-Boltzmann approach, proposed a simple electrostatic model properly including incomplete screening for the description of ferroelectric capacitors in zero and finite bias and also realized the first ever ab initio simulation of a realistic ferroelectric tunnel junction under finite bias, combining DFT and non-equilibrium Green's function formalism.

http://www.oxides.ulg.ac.be/

Project Acronym and Number: OXIDES 228989
Project Title: Engineering exotic phenomena at oxide interfaces
Start and End Dates: 01/09/2009 till 31/08/2012
EU Contribution: 2.150.000 €
Coordinator : Philippe Ghosez, University of Liège, B, Philippe.Ghosez@ulg.ac.be

Modelling

in POCO 213939

Subject of the modelling

Interactions of functionalised carbon nanotubes with polymer matrices and influence of processing parameters on different properties of the nanocomposites

Models used

Molecular Dynamics for Young's modulus of functionalized CNTs and interfacial interactions between CNTs and polymeric matrices.
Solid mechanics to obtain the elastic properties of the nanofilled composites.

Simulation software and type of numerics used

Materials Studio (Molecular Dynamics)
ANSYS Finite Elements method (FEM) for continuum mechanics
Minimization algorithms (Steepest descents, Conjugate gradient, Newton)
Ewald summation method, Finite Differences method (Verlet integrator) with Andersen numerical thermostat and barostat to simulate the NVT and NPT statistical ensembles

Achievements of the model beyond experiments

Molecular models of functionalized CNTs and polymer matrices could predict the influence of the functional groups on the mechanical properties of the CNT and the interfacial shear strength (IFSS) of the nanocomposites. The influence of the functionalization of CNTs on the IFSS of the nanocomposite was demonstrated, something that would otherwise have cost many experiments.
The pull-out of CNTs from molecular matrices is difficult to analyze by experimental methods due to the scales involved. In this case, the process modelling of the pull-out was necessary to analyze the interfacial shear strength of the nanocomposites.

Application

Polymer composites filled with CNT for automotive, aeronautics, building, aerospace, wind power generation (blades), ship building and biomedicine applications

Relevant review articles

Molecular dynamics modelling for the analysis and prediction of miscibility in polylactide/polyvinilphenol blends. de Arenaza, et al Polymer 2010 51-19 pp4431-4438
Molecular dynamics study of the influence of functionalization on the elastic properties of single and multiwall carbon nanotubes. Coto, B.et al. Comp Mat Science 2011 50-12 pp.Poly(ethylene oxide)-b-poly(L-lactide) Diblock Copolymer/Carbon Nanotube-Based Nanocomposites: LiCl as Supramolecular Structure-Directing Agent. Meyer et al Biomacromolecules 2011 12-11 pp4086-4094

Summary of the project

POCO develops innovative polymer composites filled with CNT, a nanostructured material with tailor made and superior properties. This involves development of CNT confinement strategies.

Summary of the modelling

CNTs/Polymer matrices were modelled with the following approaches for the different properties:

The influence of the functionalisation on the mechanical properties of the CNTs was analysed using a molecular dynamics approach and by calculating the stress-strain slopes.

The interfacial interactions between CNTs and polymer matrices were analysed using molecular dynamics pull-out simulations, where the interaction energy between the CNT and the polymer matrices is monitored while the CNT is being pulled-out from the matrix. This energy can be related to the interfacial shear strength.

Analytical relations were developed for the analysis of curing of the thermosetting polymers (kinetic, chemo-rheology) and used Ozawa's and Avrami's models to study the crystallization of thermoplastics semi-crystalline matrices both pure and with CNTs. For the alignment of CNTs in viscous media under electric fields, POCO developed an electro-dynamics constitutive equation relating the polarisability of the CNTs, the electric field applied and the viscosity of the polymer with the torque..

The mechanical properties such as Young's modulus, Shear modulus and Poisson's ratio of nanofilled systems have been obtained by a macromechanical model using stress-strain equations solved with a finite element approach, which was implemented in a dedicated simulation code called ANSYS.

The project has proven that a moderate degree of chemical functionalization of the CNTs can increase the interfacial shear strength up to a 300% (depending on the functional groups used) when compared to pristine CNTs.
The influence of functional groups on the properties of the CNTs has been proven to be detrimental for the mechanical properties of the SWCNTs. This detrimental effect is less critical in the case of MWCNT.

http://www.poco-project.org/home.asp

Project Acronym and Number: POCO 213939
Project Title: Carbon nanotube confinement strategies to develop novel polymer matrix composites
Start and End Dates: 01/11/2008 till 31/10/2012
EU Contribution: 5.520.000 €
Coordinator: Borja Coto, Fundacion Tekniker, ES, bcoto@tekniker.es

Modelling

in RADINTERFACES 263273

Subject of the modelling

Damage mechanisms and effects on mechanical properties for novel crystalline materials with large interfacial areas

Models used

Ab initio, molecular dynamics (MD) and continuum modeling of mechanical alloying and physical vapor deposition.
Diffusion barrier DFT, hybrid kinetic Monte Carlo-Molecular Dynamics
CFD for interface defect and dislocation mechanics

Simulation software and type of numerics used

LAMMPS Molecular Dynamics Simulator for fast and precise modelling of larger systems (multilayer systems and nanostructured systems)
Dislocation Dynamics Simulator
Finite Elements for interface motion

Achievements of the model beyond experiments

The modelling is going to guide the appropriate tuning of interfaces within multi-laminate composite materials to obtain defect absorption materials with a self-healing mechanism.

Application

Nuclear reactors, radiation damage

Summary of the project

Radiation damage is known to lead to materials failure and thus is of critical importance to lifetime of and safety within nuclear reactors. The emergence of new concepts using nanoscience in the design the design and control of nanostructures and complex defect structures can create self-healing materials for radiation-induced defects and impurities that can yield radiation impervious materials. This project aims at developing general modelling tools to predict the effect of interface composition (monophase, heterophase) and structure (geometry, roughness) on its propensity to resist radiation damage (both via defect localization and creep) using a multiscale multiphysics approach. Model validation will arise through direct comparison with materials testing for a wide array of materials systems (metal/metal, metal/oxide, oxide/oxide).

Summary of the modelling

The modelling in this project will be developed according to a multiscale multiphysics approach. First using diffusion barrier DFT and fitted many body potentials the project will quantify the energies required to activate diffusion. For the sake of simplicity, vacancies will be studied first. Ab initio simulations will be conducted on bilayer interfaces for the Cu/Nb system in the Kurdjimov Sachs orientation, for the Zr/Nb system in all three Burgers, Potter and Pistch Schraeder orientations such as to extract their excess energy and structure. Comparison with experimentally observations will serve as a validation of ab initio simulations.

Based on experimental observation and ab initio simulations of the different interface structures - such as those in the Zr/Nb system, inter-atomic potentials will be developed and improved. Atomistic models of interfaces representing bi-material interfaces (e.g. metal/metal, oxide/oxide, metal/oxide) and substrate/layer interfaces will be developed based on molecular dynamics (MD). The code will be based on LAMMPS.

A hybrid kinetic Monte Carlo-Molecular Dynamics (Object Oriented kinetic Monte Carlo) tool will be developed aiming at studying the irreversible processes taking place in the irradiation conditions at the atomic scale and in cascade events. This is done by listing all possible reactions and paths that a given defect could follow and choose the most probable one based on Monte Carlo statistical method. All possible events are quantified by migration energies, formation energies (leading to binding energies). These energies are quantified from the Nudged Elastic Band method in MD. It will be based on a newly developed synchronous parallel kinetic Monte Carlo algorithm capable of reaching longer times in larger systems and will allow following the evolution of individual defects (i.e. vacancies, interstitials, He and their clusters).

A damage accumulation model will be developed based on differential equations to describe the thermodynamic and kinetic response of the synthesized materials to microstructural features. This is 3 Dimensional Cluster dynamics model -where transport and reactions in the form of absorption and emission of defects are taken into account. Here rather than following individual defects within the nanolayered system, defect quantities are followed as densities. This leads to a great decrease in the amount of information (i.e. defects) to be followed which then allows to simulate the evolution of defect for long time scales. Discrete dislocation dynamics simulations, accounting for the symmetry of the crystals considered, will be performed to predict the mechanical response of layered systems and to extract latent hardening parameters.

At the continuum scale, interface and grain model of the interface regions will be based on point defect and dislocation mechanics concepts capable of accounting for interface morphology, diffusive processes, radiation-induced hardening, and the effect of dislocation/vacancy interactions. For example, the effect of defect penetration on the presence of disconnections (i.e. interfacial defect with both dislocation and step characters) will be considered.

A continuum mechanics based model incorporating the above constitutive models will be implemented capable of accounting for coupled diffusion-mechanical bulk and interfacial phenomena. Numerically this is going to be implemented with the Finite Element method. The code will be based on a two level approach in order to account for the coupling between interfacial motion and defect diffusion, and at each finite element time step, driving forces for interfacial motion will be calculated.

http://www.materials.imdea.org/Research/Projects/RADINTERFACES/tabid/3423/Default.aspx

Project Acronym and Number: RADINTERFACES 263273
Project Title: Multiscale Modelling and Materials by Design of interface-controlled Radiation Damage in Crystalline Materials
Start and End Dates: 01/09/2011 till 31/08/2014
EU Contribution: 3.223.002 €
Coordinator: Mohammed Cherkaoui, CNRS, mcherkaoui@me.gatech.edu

Modelling

in REFREEPERMAG 280670

Subject of the modelling

Magneto-crystalline and shape anisotropy in RE-free magnets.

Models used

Density functional theory (DFT) solving Kohn-Sham(-Dirac) equations using various basis sets, e.g., augmented plane waves with local orbitals
Micromagnetics dynamics base on the Landau-Lifshitz-Gilbert equation

Simulation software and type of numerics used

WIEN2k, Elk, muffin-tin orbitals (EMTO), pseudopotential approaches with plane waves (VASP) or numerical local orbitals (SIESTA, OpenMX). For alloys, some of the codes implement the coherent potential approximation, which is numerically rather demanding. Most of these codes provide MPI-parallel versions suitable for large-scale computations
Magnetization dynamics of magnetic particles/grains under the external field is calculated using the Landau-Lifshitz-Gilbert equation with MAGPAR, FEMME will be used together with finite element discretication codes (GID, Salome); In every iteration step the contribution of the Zeman field, the anisotropy field, and the stray field components of the particles/grains are calculated by the hybrid finite element method with boundary element method. Energy barriers for thermal switching are calculated by the implemented nudged elastic band method

Achievements of the model beyond experiments

The theory can pre-identify interesting materials prior to the actual synthesis and experiments and thus save time and resources.

Application

Magnets

Relevant review articles

Gilleien and Dronskowski • Vol. 31, No. 3 • Journal of Computational Chemistry, 2011
J. Buschbeck, et al, PRL 103, 216101 (2009)

Summary of the project

The project REFREEPERMAG aims at developing new permanent magnets (PM) with high energy product without use of rare-earths or platinum. High-aspect-ratio nano-structured materials with large magnetic moments will be studied theoretically and synthetized in environment-friendly ways.

Summary of the modelling

Two different kinds of magnetic anisotropies, namely the magneto-crystalline anisotropy and shape anisotropy are investigated. Due to their inherently different nature, they will also be studied with two different approaches. The magneto-crystalline anisotropy will be studied by first-principles electronic structure calculations. High-throughput algorithms will be employed to search the parameter-space of ternary compounds. These selected systems will be then further improved by additional degrees of freedom available through an additional alloying element.

The shape-anisotropy will be studied with a micromagnetic code based on finite element discretization in order to study the influence of realistic microstructures on the magnetic switching behaviour of nano and mesoscopic structures in order to predict optimised structures and packing densities for a nanocomposite PM. Numerical micromagnetics is a continuum approach in order to predict the hysteresis properties of mesoscopic magnetic structures including the coercive field and switching times and their thermal stability depending on the geometry and the size of the magnetic volumes.

The ultimate aim is to compact powders of magnetic nanostructures with intrinsic large coercivities.

http://refreepermag-fp7.eu/project/what-is-refreepermag/

Project Acronym and Number: REFREEPERMAG 280670
Project Title: Rare earth free permanent magnets
Start and End Dates: 01/05/2012 till 30/04/2015
EU Contribution: 3.850.000 €
Coordinator: Dr. D. Niarchos, NCSR Demokritos, Athens, Greecel dniarchos@ims.demokritos.gr

Modelling

in ROLICER 263476

Subject of the modelling

Damage and degradation of ceramics (silicon nitride, mechanical and thermal loading)

Models used

Ab initio: DFT and Mixed-Basis PseudoPotential (MBPP)
Molecular Dynamics (MD: atomistic simulations based on inter-atomic empirical potentials)
Continuum mechanics and micromechanical models for thermoelasticity, plasticity, sliding interaction, cohesive interfaces and dynamic analysis.)
Elastohydrodynamic lubrication (EHL) model (Reynolds equation)

Simulation software and type of numerics used

ABAQUS, ANSYS (FEM) and numerical methods of homogenization for continuum mechanics
Quantum Espresso for ab initio
LAMMPS for MD
EHL (Fourier analysis)
SIMPLEWARE for 3D microstructure generation

Achievements of the model beyond experiments

The FEM simulations provide solutions for micromechanical and macroscopic stress distribution in undamaged and damaged regions of components, which cannot be obtained experimentally.
The fracture models describe crack nucleation based on traction-separation laws which provide a phenomenological lifetime prediction tool without the need for extensive experiments.
The microscale models achieve homogenisation of thermoelastic properties and thermomechanical homogenisation of strengthening effects in ceramics. Such simulations provide information that cannot be obtained experimentally.
The ab initio models provide reliable properties of the bulk material and solid-solid interfaces as criteria for crack initiation, which are very difficult to obtain by experiments.
Molecular dynamics models are used in modelling hybrid steel-ceramic contact to study the interaction between additives in lubricants and bearing surfaces. Experiments that provide such information are not possible.

Application

Metalforming tools; hybrid bearings

Relevant review articles

J. Wippler, T. Böhlke, Structure and fracture property relation for silicon nitride on the microscale, Computational Materials Science, DOI 10.1016/j.commatsci.2012.02.042

Wippler, J., Fünfschilling, S., Fritzen, F., Böhlke, T., Hoffmann, M.J.: Homogenization of the thermoelastic properties of silicon nitride. Acta Materialia 59, 6029-6038 (2011) DOI:10.1016/j.actamat.2011.06.011

I. Khader, A. Hashibon, J.-M. Albina, A. Kailer,Wear and corrosion of silicon nitride rolling tools in copper rolling, Wear 271 (2011) 2531-2541.

A. Hashibon, C. Elsässer, Approaches to atomistic triple-line properties from first-principles, Scripta Materialia 62 (2010) 939-944

J.H Beynon, Finite-element modelling of thermomechanical processing, Phil. Trans. R. Soc. Lond. A, 357 (1999) 1573-158.

J.H Beynon, Tribology of hot metal forming, Tribology International 31 (1998) Pages 73-77

Summary of project

RoliCer relies on multiscale predictive models to assess damage and simulate degradation mechanisms in engineering ceramics under realistic working conditions. This will include tribology, damage analysis and lifetime predictions. The project aims at a systematic tailoring of ceramic materials for new applications, where modelling is supported by measuring techniques. The project concentrates on silicon nitride ceramics which are wear corrosion and contact fatigue resistant materials and potential materials for high temperature metal-forming tools and rolling elements for bearings

Summary of the modelling

RoliCer develops multiscale simulations based on continuum mechanics (finite-element FE numerics and numerical homogenization) and elastohydrodynamic lubrication (EHL) to predict time-dependent mechanical, tribological and thermal material stresses arising in contact. The FE simulations and micromechanical models use coupled thermal-mechanical analysis techniques to obtain material stresses as a function of material properties and realistic working conditions. Within the homogenization schemes, efficient numerical estimates of the failure probabilities depending on microstructural parameters are obtained. The modeling focuses a reliable failure prediction also for non-proportional and cyclic loading. The EHL simulations provide information on the lubrication film thickness, local stress, pressure distribution, temperature and deformation and factors affecting the breakdown of the lubrication films on real rough surfaces in mechanical contacts; the applied methodology is based on Fourier analysis of the harmonic components of the surface microgeometry to predict stresses and the induced lubricant film.

Macroscale models depend on the availability of material parameters suitable for describing the behaviour of the bulk material, and in RoliCer they are partially provided through electronic and atomistic simulations. These include the elastic constants, physical and mechanical properties of the materials involved.

First, an electronic model based on density functional theory (DFT) calculations will be conducted to investigate the adhesion of relevant metal-ceramic interfaces, and internal grain boundaries. The adhesion energy will provide direct information on the tribological aspects which relate to the degradation mechanisms. Additionally, the influence of the environment on the degradation mechanisms will be investigated. This will be achieved by considering the effects of impurities and point defects on the bonding and structure of both metal-ceramic interfaces and grain boundaries. The main assumption here is that impurities are correlated with the environment, such as (i) temperature, which enhances the diffusion and leads, for example, to higher concentration of point defects; (ii) foreign impurities originating from the metal or lubricant. As a result, the role of DFT calculations will be twofold: to investigate the correlation between the interface structure, point defects and adhesion and to provide input to the microscale simulations through constitutive equations, hence enabling the simulation of realistic working conditions.

The second atomistic method describes the interactions between atoms with semi-empirical potentials, which allow performing large-scale molecular dynamics and static relaxation. Such methods can be used to study large scale defect structures in the ceramics, such as dislocations and general incoherent grain boundary models.

The effect of temperature, or thermal stresses will be studied large-scale molecular dynamics and static relaxation; two distinct approaches will be tackled, by inducing large thermal gradients, or via coupling to statistical physics (fluctuation-dissipation theorem) where one can estimate the rate of thermal transport, and its effect on the degradation of the materials, for example, through the interaction of dislocations and phonons (which are the means by which the thermal energy is transported in the system).

The initiation and propagation of cracks will be investigated efficiently using molecular dynamics and static (relaxation of atomic positions at absolute zero temperature) simulation techniques. Such simulations require reliable interatomic potentials. Constitutive equations will also be derived from the results of the interatomic potentials, which would have the advantage of dealing with incoherent interface models, and take temperature effects into account as well.

http://www.rolicer.eu

Project Acronym and Number: ROLICER 263476
Project Title: Enhanced reliability and lifetime of ceramic components through multiscale modelling of degradation and damage
Start and End Dates: 01/12/2011 till 30/11/2014
EU Contribution: 2.600.000 €
Coordinator: Andreas Kailer, Fraunhofer Institute for Mechanics of Materials IWM;
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Modelling

in SIMBA 229034

Subject of the modelling
Synthesis of silicon nanopowders in Inductively Coupled Plasma (ICP) systems

Models used
Computational Fluid-Dynamics (CFD) for plasma physics, precursor evaporation and nanopowder transport and growth
Chapman-Enskog method for plasma thermodynamic and transport properties

Simulation software and type of numerics used
Commercial CFD code ANSYS FLUENT extended to take into account plasma physics, precursor evaporation and nanopowder synthesis.
Numerical routines written in C for the Chapman-Enskog method to calculate plasma thermodynamic and transport properties needed in CFD simulations.

Achievements of the model beyond experiments
The modelling of the plasma flow dynamics and particle trajectories permitted to define the process at different scales and to predict the influences of the main process parameters (e.g. effects on nanopowder production yield when changing the reactor geometry and operating conditions).
The model enabled the design of an optimum reactor chamber with increased flow of particles for collection thus avoiding an expensive try-and-fail approach, and saving time and effort in optimising the lab scale process and in transferring main results to an industrial ICP installation.

Application
Production of anode material (nano-silicon based) for Li-Ion battery and photovoltaic applications

Relevant review articless
Colombo V et alii, Two-temperature thermodynamic and transport properties of argon-hydrogen and nitrogen-hydrogen plasmas, Journal of Physics D: Applied Physics 42 (5), 2009
Colombo V et alii, Three-dimensional investigation of particle treatment in a RF thermal plasma with reaction chamber, Plasma Sources Sci. Technol. 19 (2010) 065024
Colombo V et alii, A three-dimensional investigation of the effects of excitation frequency and sheath gas mixing in an atmospheric-pressure inductively coupled plasma system, J. Phys. D: Appl. Phys. 43, 105202 - 105214 (2010).
Colombo V et alii, 3-D Time-Dependent Large Eddy Simulation of Turbulent Flows in an Inductively Coupled Thermal Plasma Torch with Reaction Chamber, IEEE Trans. Plasma Sci, 6th Triennial Special Issue on Images in Plasma Science, 2011.
Colombo V et alii, Two-dimensional nodal model with turbulent effects for the synthesis of Si nano-particles by inductively coupled thermal plasmas, Plasma Sources Sci. Technol. 21, 025001 (2012)

Summary of the project

The project SIMBA addresses the upscaling of synthesis of metallic nanoparticles with the Inductively Coupled Plasma (ICP) technique. This project developed an industrial production line including on-line monitoring systems for silicon and silicon-based alloyed nanoparticles, which can be applied as anode material in battery applications. It included an on-line functionalisation technique and an industrial powder injection system to ensure a continuous production.

Summary of the modelling

An advanced CFD model FLUENT (including electromagnetics, non-LTE effects, chemical non equilibrium, turbulence models, discrete-phase model with plasma-particle interaction, plasma thermodynamic and transport properties) was used in SIMBA. This code uses parallel computing, and is capable of capturing the fine geometric details. The existing model can predict temperature and flow fields of different plasma mixtures of a variety of gases together with injected particle temperature and trajectory prediction. This model for plasma fluid-dynamics has been extended to simulate non-equilibrium plasma (low pressure operating conditions and the strong temperature gradients due to the quenching system) and for the nanopowder nucleation out of the gas phase (aerosol model to track the particle size-distribution and particle population in the reactor region and to calculate process yield). A model for the precursor particle thermal history and trajectory prediction as well as nanoparticles production has been developed.

The model is applied to the actual lab-scale Empa reactor (plasma torch and reaction chamber) and has been proven to calculate temperature, velocity, viscosity profiles of plasma flow in the whole system. The model has been validated through comparison with enthalpy probe measurements of temperature under different operating conditions and calorimetric measurements for energy balance of the plasma system. The computational effort of this calculations is reduced by a) limiting the computational domain to the most important regions of the reaction chamber (e.g.: the quenching zone); b) decoupling the plasma torch with the reaction chamber domain, using the calculated plasma torch outflow fields (temperature, velocity, concentration, ...) as boundary condition for the reaction chamber.
The model has allowed a design-oriented modelling approach to optimize the lab scale process and then to transfer main results to an industrial ICP installation.

www.simba-project.eu

Project Acronym and Number: SIMBA 229034
Project Title: Scaling-up of Inductively Coupled Plasma technology for continuous production of Metallic nanopowders for Battery Applications
Start and End Dates: 01/9/2009 till 01/08/2012
EU Contribution: 2.869.275 €
Coordinator: Stijn Put, Umicore, BE, stijn.put@umicore.com

Modelling

in SIMUGLASS 233524

Subject of the modelling

Precision glass moulding

Models used

Model for precision glass moulding process including:
- Elastic model (for mould)
- Visco-elastic models (for glass)
- Ideal gas model (for protection gas)

CFD for gas model: Navier–Stokes equations (continuum equation, momentum equation and thermal equation), conduction, convection, radiation
Continuum Mechanics model: Hooks law, General Maxwell equation, Kelvin equation, Burgers equation, Newton's fluid, WLF shift function, Narayanaswamy equation

Simulation software and type of numerics used

ABAQUS, ANSYS (Finite Element codes)
Transient solving, implicit method

Achievements of the model beyond experiments

Shape of moulds can be now predicted with the help of modelling of the glass shrinkages, which had to be done previously by expensive try-out experiments.
Index drop inside glass lens can be now predicted with the help of modelling of the structure relaxation behaviour of glass material, which was unknown only by pure experiments.
Material flow and temperature during forming process can be predicted, which can not be observed and measured in the real moulding process.

Application

Optics for lighting and photovoltaic
Optics for imaging
Optics for laser apparatus

Relevant review articles

O. Dambon, F. Wang, Y. Chen, A. Y. Yi, F. Klocke, G. Pongs, "Efficient Mould Manufacturing for Precision Glass Moulding," J. Vac. Sci Technol. B, 27 (3), 1445-1449 (2009).
A. Jain, A. Y. Yi, X. Xie, R. Sooryakumar, "Finite Element Modeling of Stress Relaxation in Glass Lens Moulding Using Measured, Temperature-Dependent Elastic Modulus and Viscosity Data of Glass," Model Simul Mater SC, 14 (3), 465-477, Mar (2006).

Summary of the project

This project has developed a FEM-tool for material modelling, process simulation and optimization of optical glass moulding. The relevant thermal, mechanical, rheological and optical glass material properties and their dependence on the moulding parameters (forming velocity, temperature, force, etc.) were investigated.

Summary of the modelling

The simulation of hot glass deformation is a complex thermo-mechanical problem comprising interactions between radiative/conductive thermal transport phenomena, incompressible, viscous fluid dynamics of softened glass and the large strain/large displacement visco-elastic/visco-plastic deformation of glass due to pressing in the mould.
Some of the important issues to be addressed by modelling are (a) large free surface deformations (b) complex contact phenomenon (c) high deformation rate (d) time and temperature dependent boundary conditions and (e) high degree of material non-linearity

The project has developed a generalized simulation tool covering the whole cycle of glass moulding for the whole relevant temperature range incl. newly developed glass material models.

The structural mechanics code is based on the commercial packages MARC, DEFORM 3D, FIDAP, POLYFLOW, SYSTUS, ANSYS, ABAQUS, and LS-DYNA. The project developed a CFD model for the behaviour of the laminar flow of the protection gas, which is usually nitrogen gas. Such protection gas is used only not to prevent the heated glass material from being oxidised, but also to help the heat flow convect more efficiently inside the machine chamber. , This is used to determine the thermal boundary conditions for the FEM model of the glass forming process. New glass material model for the thermo-rheologically viscoelastic material behaviour, which occurs in the moulding process, is developed based on existing models like Hooks, Maxwell, Kelvin, Burgers fluid, Newton's viscosity materials model, in which the strain rate and time dependency is considered.

The result is a complete process simulation including structural and thermal analysis, which covers all the important procedures during the moulding process: heating, soaking, moulding, holding and cooling.

www.simuglass.com

Project Acronym and Number: SIMUGLASS 233524
Project Title: Development of a Synergistic Computational Tool for Material Modeling, Process Simulation and Optimization of Optical Glass Moulding
Start and End Dates: 01/01/2010 till 31/12/2013
EU Contribution: 899.994 €
Coordinator: Dr. Olaf Dambon, Fraunhofer Institute for Production Technology IPT,
olaf.dambon@ipt.fraunhofer.de

Modelling

in SMASH 228999

Subject of the modelling

GaN nanocolumn LEDs

Models used

Quantum mechanical models for eigenstates of confined particles in nanostructures both at continuous media (EFA k·p) and atomistic (empirical tight-binding) level
Semiclassical electron and hole transport models
Modelling of strain in heterostructures with linear elastic continuum mechanics and valence force field method (VFF)

Simulation software and type of numerics used

TiberCAD for strain/electronic modeling
QUATRA/CELS for luminescence modeling
Numerical libraries, such as portable extensible toolkit for scientific computation and scalable library for eigenvalue problem computations (PETSc, SLEPc)

Achievements of the model beyond experiments

The modelling and simulation of GaN-based LEDs is able to guide the device design, by optimizing strain, polarization and quantum effects in order to improve the performance of the devices. Atomistic simulations can shed light on the effect of clustering in the alloy active regions.

Application

LEDs

Relevant review articles

Auf der Mau, M et al; IEEE TRANSACTIONS ON ELECTRON DEVICES, Vol. 58, No. 5, May2011, overview on the multi-scale approach is given, and on what is essential to simulate the growth and the electro-optic properties of nanowires.

Summary of the project

The project SMASH has developed LEDs of high efficiency and low cost. An epitaxial growth technique based on nano-rod coalescence on ultra-low defect density templates has been realised. Also growth of directly emitting Gallium Nitride based nano-rod structures has been developed. High efficiency devices covering the entire visible spectrum and phosphor-free white LEDs have been manufactured.

Summary of the modelling

The multiscale simulation tool TiberCAD includes all the relevant physical models, both at continuous and atomistic level, for the investigation of strain, transport and optoelectronic properties of GaN nanocolumn structures.

The calculation of strain in lattice mismatched heterostructures is based on linear elasticity theory of solids, assuming pseudomorphic interfaces between different materials. Transport of electrons and holes is treated in a semi-classical picture based on the drift-diffusion model. The particle fluxes are written in terms of the electrochemical potentials. The carrier statistics are given by Boltzmann or Fermi-Dirac statistics, assuming as usual local equilibrium. The conduction and valence band edges and effective masses are obtained from bulk k·p calculations, which include the local corrections due to strain. Quantum mechanical models used for the calculation of eigenstates of confined particles in nanostructures, are based on the envelope function approximation (EFA) and on the empirical tight binding (ETB) method. In the first case, the Hamiltonian of the system is constructed in the framework of single-band and multiband k·p theory. The ETB method is an atomistic approach where electronic states are written as a linear combination of atomic orbitals (LCAO). The atomistic structure, which is needed for ETB calculations, is generated internally in TiberCAD according to the macroscopic device description and crystallographic orientation. Strain maps and the effects of strain, piezo and spontaneous polarizations, as well as surface states, on band profiles have been studied in GaN nanocolumn p-i-n diode structures with different active regions, such as Quantum Disk (QD) and Core Shell. Electron and hole states of the QD have been calculated, both with an EFA k·p model and an empirical tight-binding (TB) atomistic model. Self consistent band profiles have been calculated by concurrently solving the Poisson/drift-diffusion and the quantum mechanical models. Optical emission spectra and the dependence of transition energies on geometrical and material parameters have been found.

Carrier capture and escape in and out of the well is described with a combination of a drift-diffusion model in the contact region and more sophisticated quantum description in the region close to the quantum well is used. Electroluminescence spectra are obtained with a custom developed quantum kinetic model (CELS/QUATRA).

Optical properties of nanorods, in particular the extraction efficiency, emission directionality and polarization, are calculated with the electromagnetic simulation tool OptiWave. The microscopic complex refractive index is taken as input, as well as the different absorption by metals and semiconductors. The wave guiding properties of a single nanorod, as well as the electromagnetic coupling of the rod arrays forming a collective photonic crystal emitter or bottom distributed reflector are investigated, and an optimum design is developed.

Coupled electro-optical properties in a LED device are studied by applying a combination of the described above. Exciton and carrier distributions, polarization states of emitted photons, radiation characteristics are calculated also by finite element tools FDmax and CELS/QUATRA. Finally, key device specifications such as the internal and external efficiency of nanorods in LED geometries are simulated and structure parameters for an optimized LED performance are determined. In particular, the design for phosphor-free white light emitting devices is optimized, which is crucial to meet specific colour coordinates. The model results have been used as input to adjust epitaxial growth conditions and stamp design.

www.smash-fp7.eu

Project Acronym and Number: SMASH 228999
Project Title: Smart Nanostructured Semiconductors for Energy-Saving Light Solutions
Start and End Dates: 01/09/2009 till 31/8/2012
EU Contribution: 8.299.360 €
Coordinator: Martin Strassburg, OSRAM Opto Semiconductors GmbH, DE, martin.strassburg@osram-os.com

Modelling

in SSEEC 214864

Subject of the modelling
Magnetic materials, micromagnetism, magnetic cooling engines

Models used
Ab initio DFT models of non-collinear magnetic material groundstates (electronic quantum mechanical models using 10s of atoms)
Preisach model of hysteresis (irreversibility) in phase transformations at the mesoscale.
Micromagnetic (mesocale) models, including exchange-coupled nanocomposites (1-10 nm)
Magnetic cooling engine prototypes: continuum modelling of materials including conductive and convective heat equations, Maxwell equations and fluid dynamics equations.

Simulation software and type of numerics used
Ab initio DFT models: OpenMX (http://www.openmx-square.org/) and VASP (http://www.vasp.at/). Site-based magnetic moments were calculated using the Voskown analysis within the general gradient approximation scheme.
Preisach model of hysteresis: original C++ code written and solved in-house.
Micromagnetics: Free energy of a magnetic solid, solved using in-house C++ code.
Magnetic cooling engine prototypes: COMSOL Multiphysics, Matlab, Mathematica. Finite element and analytical treatments were used. The entropy generation method was developed for efficiency analysis.

Achievements of the model beyond experiments
The materials modelling gave us invaluable feedback on experimental development, reducing the time that would otherwise be required to make multiple measurements or a full phase space of physical samples.
Regarding the cooling engines, the 2D model of an active magnetic regenerator (AMR) enabled accurate optimisation of geometry (packing density, absolute length scales), system operating parameters (frequency, flow rate) and identification of optimal (or ideal) refrigerant material properties (magnetocaloric effect and heat capacity) against overall efficiency and power requirements.

Application
Magnetic materials, manufacturing industry, magnetic cooling engines

Relevant review articles
The papers containing the DFT work are:
Barcza, Gercsi, Knight and Sandeman, Phys. Rev. Lett. **104** 247202 (2010)
Gercsi and Sandeman, Phys. Rev. B. **81**, 224426 (2010)
Gercsi, Hono and Sandeman, Phys. Rev. B. **83**, 174403 (2011)
Micromagnetics: Basso, J. Phys. Condens. Matt. **23** 226004 (2011).
Reviews: “Gas-free refrigeration” K.G. Sandeman, Magnetics Technology International, **1** 30 (2011); “Magnetocaloric materials: the search for new systems” K.G. Sandeman, Scripta Materalia **67** 566-571 (2012)

Summary of the project

The ultimate goal of this project was to lower the economic barrier to entry of magnetic cooling as a high efficiency cooling technology free from greenhouse gas refrigerants. SSEEC's efforts in this direction centred around the development of a low power heat pump based on a highly efficient magnetic refrigeration cycle. The device features a magnetic refrigerant that is magnetised and demagnetised by movement relative to a permanent magnet. The core materials research concerned the identification, synthesis, modelling and production of low cost, environmentally friendly magnetic refrigerant materials based on new (nano)-architectures.

Summary of the modelling

SSEEC aimed to develop an integrated approach to magnetic cooling for an end-user application. This entailed characterisation of materials, integration of those into prototype cooling engines, and integration of those engines into an end-user (heat pump) system. The modelling work examined magnetic refrigerants (novel physical mechanisms of magnetic cooling) and magnetic cooling engines (an integrated view of the impact of design on cost and performance).

Magnetic refrigerants: DFT models were used to calculate site-based magnetic moments using the Voskown analysis within the general gradient approximation scheme. Giant magneto-elastic coupling in CoMnSi (a metamagnetic refrigerant material) and thereby the dependence of magnetism on Mn-Mn interatomic distance in Mn-based materials of the same structure (*Pnma* space group) was modelled as it can be used to understand and control magnetic phase transitions. This modelling led to predictive synthesis of new metamagnets.

The exchange coupling between the phases in the composite material were calculated (note this is at nano-scale). It was found that the entropic, or cooling effect of a nano-scale spin reorientation-based refrigerant is diluted by any amount of second, exchange-coupled phase, and that, for the oxide systems synthesised, retention of a single phase is more desirable. However, for other systems a second phase could be of use in broadening the temperature range of use of a candidate refrigerant.
Micromagnetics models used exchange couplings, dependent on composite geometry, as an input. First the effect of mixing a spin reorientation material with a ferromagnet in a nano-composite in which the constituent phases were exchange coupled was modelled. It was demonstrated that the total entropy change of the composite was reduced, but spread over a wider temperature range. Secondly a nano-scale magnetic heterostructure comprised of two different hard magnetic materials with orthogonal axes of unaxial anisotropy was designed and proved to function as a theoretical anisotropy switch, the optimal dimensions of which were determined by the composition of each layer.

Magnetic cooling engines: different cooling cycles were modelled using "real" magnetic materials that have magnetic phase transitions (required for magnetic cooling) which exhibit magnetic hysteresis (a source of loss). Experimental data were used to generate a detailed picture of the magnetic cooling effect of La-Fe-Si when deployed in a relevant, "regenerative" cooling cycle.

Cooling engine modelling underpinned a comprehensive design approach for the development of magnetic cooling engine prototypes, including the different aspects at work within a magnetic cooling engine: material properties, heat transfer, fluid flow, magnetic fields and loss processes, as well as optimising the design of individual components. Various system components were modelled. Over 100 magnet designs were examined and tuned, valves were optimised for flow, pressure drops and flow rates, and magnetic forces inside the cooling engine (both regenerators and magnetic valves) were optimised. Accurate optimisation of an overall system design that can meet the power, weight, span, volume and cost targets needed for a commercial system was achieved.

http://www.sseec.eu

Project Acronym and Number: SSEEC 214864
Project Title: Solid State Energy Efficient Cooling
Start and End Dates: 1/12/2008 till 31/11/2011
EU Contribution: 1.885.534 €
Coordinator: Karl G. Sandeman Imperial College London UK k.sandeman@imperial.ac.uk

Modelling

in SUPER-IRON 283204

Subject of the modelling
Physical properties of iron-pnictides superconductors (spin susceptibility and effective electron-electron interaction) in superlattices, thin-films, interfaces, grain or twin boundaries.

Models
Various Density Functional implementations
Classical molecular dynamics
Bogoliubov-de Gennes model for the superconducting and magnetic phases

Simulation software and type of numerics used
All-electron codes (Fleur, Elk and FLAPW)
Plane-waves implementations (VASP, Quantum-Espresso)
Local basis, linear scaling DFT codes (Siesta, OpenMX)
The DFT implementations are all stable, optimized, parallelized and highly maintained codes. They are mainly based on complex matrix manipulations and Fast Fourier Transform operations.
Specific developed software will be based on iterative matrix diagonalization and many-body multiband Hamiltonian solution.

Achievements of the modelling beyond experiments
Prediction of high-pressure phase transitions in $Ba(Ca)Fe_2As_2$ and of non-hydrostatic effect, confirmed by high-pressure XRD measurements.
Prediction of the peculiar structural and electronic modification upon doping with rare-earth metals in $CaFe_2As_2$.
Understanding of disorder, surface and interface effects.
Model calculations, joined with DFT calculations, were able to predict a tri-critical point in the phase diagram of iron-pnictides, now a hot subject for experimental confirmation.

Application
Non-conventional iron-based superconductors systems

Relevant review articles:
M.Putti, et al., “New Fe-based superconductors: properties relevant for applications” Supercond. Sci. Technol. **23** (2010) 034003
K. Tanabe and H. Hosono “Frontiers of Research on Iron-Based Superconductors toward Their Application” Japanese Journal of Applied Physics **51** (2012) 010005
G. R. Stewart “Superconductivity in iron compounds” Reviews of Modern Physics, **83** (2011) 1589

Summary of project

The topic is to investigate Fe-based superconductors characterized by FeAs (or FeSe) planes separated by different layers. Among these compounds there are the so called 1111 phase (represented by the LaFeAsO), the 122 ($BaFe_2As_2$), the 111 (LiFeAs) and the 11 (FeSe) phases as well as the new pnictide oxide superconductors intercalated by oxides blocking layers. Superconducting properties will be investigated also under high magnetic field and/or pressure and visualization of local electric field and current will be carried out with a number of techniques. SUPERIRON will then depict the roadmap for exploring and exploiting the potentialities of Fe-based superconductors (FeSC).

Summary of the modelling

SUPER-IRON will use models to predict structural, electronic and superconducting properties of interfaces in FeSCs. In particular, they will study: single crystal properties (superlattices), the interface between two layers of the same material but with differently oriented crystalline axes and properties of interfaces between two different materials (blocking layers, superconductor/metal interface).

Bulk samples of single crystals will be simulated with parameter free first-principles simulations (Density Functional Theory, DFT). The effect of substitutions, various kinds of defects and applied pressure on the structural, electronic, magnetic and superconducting properties of FeAs superconductors will be investigated. This will provide input parameters for multiband analyses of superconducting and normal state properties.

Interface properties will be simulated by first-principles structural models. The study will address layers with misoriented crystalline axes, the stability and energetics of thin film geometry and superlattices formed by different layers of various FeAs superconductors. Lattice mismatch, uni-axial pressure effects, interface and surface states will be investigated.

Also the possibility of incorporating perovskite and metal blocking layers intercalated with FeAs planes will be studied. The structural stability of the terminations, defect formations and their effect on the electronic, magnetic and superconducting properties will be predicted.

The interplay of temperature and pressure, structural and magnetic transition will be studied by Landau theory developed from ab-initio calculations fully taking into account the effect of the crystalline structure.

Effective tight-binding Hamiltonians will be constructed starting from first-principles to describe the electronic properties of defects, superlattices and grain boundaries and simulate the superconducting properties (Jc, Hc, Tc) by means of Bogoliubov-De Gennes equations. This will give information on the superconducting properties: order parameters in real space across the boundary, superconducting current flow at the boundary and critical currents (Jc° and how the superconducting properties of FeSCs are affected by the mis-orientation angle will be predicted.

First-principles models of effective interactions between electrons, including spin fluctuations, will be elaborated to provide fundamental information on the superconducting transition, and its dependance on the critical temperature. The calculation of superconducting properties will be done extending the ab-initio SuperConducting Density Functional Theory with electronic pairing interactions.

A different crystallographic orientation of the grains and different properties of the grain boundaries result in a strongly inhomogeneous current flow. A model, based on an approach for percolation in MgB_2, will be developed, which predicts loss-free macroscopic currents.

http://www.super-iron.eu/

Project Acronym and Number: SUPER-IRON 283204
Project Title: Exploring the potential of iron-based superconductors
Start and End Dates: 01/10/2011 till 30/09/2014
EU Contribution: 1.725.659 €
Coordinator: Marina Putti, CNR-SPIN, putti@fisica.unige.it

Modelling

in SUPERLION 214832

Subject of the modelling

Nano-architectured battery materials and 3D microbattery components.

Models used

Molecular Dynamics(MD) for electrochemical phenomena for material/battery/production process optimization
Lattice Gas Model for charge and mass transport

Simulation software and type of numerics used

Comsol Multiphysics is also used for the flow and electrochemical phenomena DL POLY and MCGEN for nanoscale battery architecture

Achievements of the model beyond experiments

The model allowed shortened and better-informed selection of the most efficient cell architectures and geometries, and the optimal cell materials. Modelling can avoid excessive and often futile efforts to create more impressive micro-architectured electrodes, since these will often not result in improved battery performance.

Application

On board microbatteries for electronic and medical devices.

Relevant review articles:

Kasemägi et al., Solid State Ionics, 168 (2004) 249
Brandell et al., J. Mater. Chem., 15 (2005) 4338.
Thomas et al., ECS Meeting Abstracts, Los Angeles, Oct. 2005.
Thomas et al., Modelling studies of 3D-Microbatteries, IMLB-13, Biarritz, May 2006.
Liivat et al., Polymer, doi: 10.1016/j.polymer.2007.08.05
Liivat et al., J. Mater. Chem., doi:10.1039/b706938c.

Summary of the project

The project SUPERLION has contributed to improved materials synthesis, and the design and fabrication of novel 3D nano-architectured microbattery components.

Summary of the modelling

Atomic-scale Molecular Dynamics (MD) modelling of branched PE/PEO as a host matrix for Li-ion battery electrolytes, and electrochemical and transport modelling with Finite Element (FE) modelling is made of the individual materials considered for relevant battery architectures and geometries.

Electrochemical system modelling (with the code Comsol) has provided new and invaluable insights into the optimal device configurations, given the technological and materials limitations. A first approach exploiting Newmann theory has simulated the porous electrodes in prospective micro-scale Li-ion batteries and has given current-voltage relationships for the complete 3D-MB device. This work has provided valuable input for material/battery/production process optimisation.

This approach has been accompanied by simulation of charge and mass transfer in the 3D-MB structures. The description of equilibrium potential of the electrode material has been based on the Lattice Gas Model with COMSOL. Diffusion of Li ions inside the electrode material is simulated by numerically solving the relevant diffusion equations for appropriate geometries. Simulation of electrolyte phenomena has been made by applying the Nernst-Planck approximation.

Simulations of complete 3D-MB geometries are done at both an atomic- and continuum-level to better understand the underlying reasons for critical current distributions within micro-/nano-micro-battery systems. Work at both levels is needed in understanding the basic functionality/design relationships in 3D micro- and nanoscale battery architectures. MCGEN and DL_POLY are software codes used for atomic-scale polymer MD and COMSOL is used for FEA modelling of 3D-microbattery architectures.

www.superlion.eu

Project Acronym and Number: SUPERLION 214832
Project Title: Superior Energy and Power Density Li-Ion Microbatteries
Start and End Dates: 01/9/2008 till 31/08/2011
EU Contribution: 2.800.000 €
Coordinator: Josh Thomas, Dept. of Chemistry, Uppsala University, Sweden, Josh.Thomas@kemi.uu.se

Modelling

in SURFUNCELL 214653

Subject of the modelling
Adsorption phenomena at the interface of cellulose surfaces

Models used
Atomistic modelling of cellulose/water interface with molecular mechanics (MM) using the GLYCAM06 force field (supercell approach with periodic boundary condition).
Atomistic modelling of hydrogen bonding and dispersion interaction between cellobiose and glucose with DFT and DFT-D, Coupled-Cluster (molecular approach).
Coarse grained, grid-based model of the interaction of nanoparticles among each other and with cellulose substrate, implemented using own software developed for the project.

Simulation software and type of numerics used
Molecular mechanics (MM) using the GLYCAM06 force field. Programs: ChemShell, DL_POLY
DFT and DFT-D, functionals used: BP86, B3LYP, M06
QC programs: TURBOMOLE, TERACHEM

Achievements of the model beyond experiments
Modeling reproduced and predicted the strength and structured buildup of hydrogen bonds of water to the cellulose surface and inside the water layer as a function of the water layer thickness. This led to suggestions for the design of the surface structure and charge distribution at cellulose surfaces.

Application
Interfacial chemistry

Summary of the project

The aim of the project is the creation of functional surface modifications using polysaccharides and nano-particles leading to four different demonstrators in the fields of pulp and paper, cellulosic yarns, cellulose films and filter membranes.

Summary of the modelling

Adsorption of water or small or large carbohydrates on cellulose surfaces is frequently attributed to the formation of highly stable hydrogen bonds. Adsorption phenomena at the interface of cellulose surfaces require modeling of a system that is composed of two subsystems: the cellulose bulk and the adsorbate. The modelling of the interaction between cellulose and water using force fields is very delicate: water-water interaction in bulk water can be described with water models, which are not part of the force fields used for cellulose. Therefore the modelling of the interaction at the interface has to be considered as crucial and this can only be done by comparing results at different level of theory (quantum mechanical and molecular mechanics methods).

Within the Surfuncell project, a study was started with classical molecular dynamics using CHEMSHELL and DL-POLY on the strength of different H-bonds in cellulose, separating the intrinsic H-bond dissociation energy (H-bond strength) from the atom-pair van der Waals interactions. The interaction of cellulose surface of different morphologies and any kind of adsorbates as a function of the water layer thickness using molecular dynamics simulations was also studied to get a feeling for the number of water molecules that are necessary for the adsorption of solvated molecules at the cellulose surface.

Coarse grained modelling within house codes was used to simulate the formation of layers of nanoparticles on cellulose surfaces. For this purpose, a grid-based, discrete model operating at the scale of the nanoparticles has been developed. The model assumes a simplified geometry of the particles, a limited discrete set of particle locations and orientations and a simplified, short ranged interaction between particles and the surface. In return, this coarse-grained approach allows the simulation of layer formation involving millions of particles and a subsequent analysis of the layers' statistical properties.

www.surfuncell.eu

Project Acronym and Number: SURFUNCELL 214653
Project Title: Surface functionalisation of cellulose matrices using coatings of functionalized polysaccharides with embedded nano-particles
Start and End Dates: 01/12/2008 until 30/11/2012
EU Contribution: 7.916.259 €
Coordinator: Prof Volker Ribitsch Uni Graz, AT volker.ribitsch@uni-graz.at

Modelling

in ULTRAMAGNETRON 214469

Subject of the modelling

Optical control of nanomagnets (rare earth transition metals, diluted magnetic semiconductors) including reversal and (thermal) relaxation

Models used

Electronic modelling of the ultrafast laser-induced magnetization reversal based on the use of the Heisenberg formalism for the exchange interaction between atomic spins.
Atomistic modelling of a ferrimagnetic material with magnetic compensation points
Landau-Lifshitz-Bloch (LLB) equation
LLB based multi-macro spin simulation for magnetisation of nanodot arrays

Simulation software and type of numerics used

Parallel version of the codes

Achievements of the model beyond experiments

Materials with a compensation point are shown to be very promising media for magnetic recording.
The magnetization reversal by a single circularly polarized laser pulse has been successfully simulated
A phase diagram for opto-magnetic reversal was obtained, demonstrating a window of peak electron temperature and effective magnetic field pulse duration for opto-magnetic switching
A new mechanism of linear magnetization reversal was discovered
Experimentally the two sublattices of a ferrimagnetic alloy (GdFeCo) were found to demagnetise at different rates which was then confirmed by the model
The model predicted that the ferrimagnet transitioned into a transient ferromagnetic phase stable for only around 300femtoseconds which was found experimentally (Nature 2011)
The theoretical model predicted that the magnetisation of the ferrimagnet reversed spontaneously on application of a heat pulse, which was then experimentally verified (Nature Comm.2012)

Application

THz magnetic recording and information processing devices
(opto-magnetic read-head and the required picosecond laser and write heads)

Relevant review articles

Nature, 472, 205 (2011); Nature Communications 3, #666 (2012)

Summary of the project

The objective of the EU-India project was to develop “opto-nano-magnetism” that is, the manipulation of the magnetic properties of nanomagnetic materials with light using (magneto-) optical effects, as a novel approach for future magnetic recording and information processing technology. This topic is situated at the junction of coherent nonlinear optics, nanophotonics and magnetism. In particular, we investigated the effects of light on magnetic order at the nanoscale, optimized materials and conditions for highly efficient and ultrafast (10-12 seconds and faster) optical control of nanomagnets and in this way tried to initiate a development of novel technology for unprecedented fast (THz) magnetic recording and information processing.

Summary of the modelling

Models have been developed for the physical understanding of the opto-magnetic process. The models have given an understanding of the thermal processes involved in the opto-magnetic reversal process. The electronic model is based on the use of the Heisenberg formalism for the exchange interaction between atomic spins. It is demonstrated that ultrafast reversal can occur on heating close to the Curie temperature in the presence of a large applied field
After establishing the basic physics of the reversal detailed calculations were carried out using a model based on the Landau-Lifshitz-Bloch (LLB) equation. The LLB equation has the property that the magnetisation is not conserved which means that it can be used in calculations at elevated temperatures up to and even beyond the Curie temperature. In a single spin approximation, the LLB equation is computationally efficient and the influence of a magnetic field on the recovery phase following a rapid heat-pulse was investigated. This field originates in the laser-pulse due to the inverse Faraday effect.
The micromagnetic modelling is applied to ferrimagnetic material such as GdFeCo. Ferrimagnets have a magnetic compensation point which may contribute to the ultrafast reversal. It is important to study the dynamics of ferrimagnetic materials in order to understand their ultrafast dynamic magnetisation properties. For the modelling of laser-induced magnetization reversal at the nano level opto-magnetic switching processes of a single macro-spin in the framework of the Landau-Lifshitz-Bloch (LLB) equation recently derived by D. Garanin [Phys. Rev. B 55, 3050 (1997)] was investigated. It was found that the maximal electron temperature, as well as the field pulse duration, influence the reversal of the magnetic system. These findings coincide with observations found experimentally. Furthermore, it has been shown numerically as well as experimentally that the occurring reversal is not precessional in nature, but has instead a linear character, proceeding via a strongly-nonequilibrium state. The so-called linear reversal mode previously investigated analytically for a single LLB macro-spin leads to reversal processes on an ultra-short time scale. The next step went beyond this single-macro spin approach and extended the approach to a LLB based multi-macro spin simulation. The exchange coupling as well as the dipolar interaction were taken into account. Here, the long-range dipole-dipole interaction is calculated with the aid of the well-established fast-Fourier transformation (FFT). Furthermore, the code was paralellised in order to simulate extended systems of realistic size up to 107 macro-spins on our computer cluster at Konstanz.
With these new programs, systems were simulated with up to 4*106 macro-spins. A Gaussian electron temperature profile was assumed in order to model a realistic laser spot as used in the experiments. The magnetization evolution corresponds to those found in the experiment.

Project Acronym and Number: ULTRAMAGNETRON 214469
Project Title: Ultrafast all optical magnetization reversal for magnetic recording and laser controlled spintronics
Start and End Dates: 01/12/2008 till 31/11/2011
EU Contribution: 3.147.150 €
Coordinator: Theo Rasing Radboud University NL th.rasing@science.ru.nl

Annex II
List of software codes used

SOFTWARE	*where they are used by the NMP projects*	*website*
ABAQUS	Continuum solid mechanics (micro and macro); fluid dynamics; process	www.3ds.com/fr/products/simulia/portfolio/abaqus/overview
ABINIT	Electronic: quantum mechanical	www.abinit.org
ACEFEM	Continuum solid mechanics (micro and macro)	www.wolfram.com/products/applications/acefem
ADF	Electronic: quantum mechanical and and many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods	www.scm.com/Products/ADF
AMBER	Atomistic: ab-initio molecular dynamics and Quantum Mechanics/Molecular Dynamics	www.ambermd.org
AMPAC	Electronic: quantum mechanical and many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods	www.semichem.com
ANSYS (FLUENT)	Continuum solid mechanics (micro and macro); fluid dynamics	www.ansys.com
ANSYS HFSS	Continuum: Electomagnetism	www.ansys.com
BOLTZTRAP	Electronic: many-body and semi-empirical or parametrised electronic models	www.icams.de/content/departments/ams/madsen/boltztrap
CANTERA		code.google.com/p/cantera
CASTEP	Electronic: quantum mechanical and Atomistic: ab-initio molecular dynamics and Quantum Mechanics/Molecular Dynamics	www.castep.org
CHEMKIN	Continuum: chemistry	www.reactiondesign.com/products/open/chemkin
CHEMSHELL	Continuum: chemistry	chemcell.sandia.gov
CFX ANSYS	Continuum: fluid mechanics	www.ansys.com/Products/Simulation+Technology/.../ANSYS+CFX
CODICE_DEG	Continuum: solid mechanics (micro)	www.codice-project.eu/codes and demos
CODICE_MEC	Continuum: solid mechanics (micro)	www.codice-project.eu/codes and demos
COM-FIRE	Continuum: solid mechanics and chemistry	Inhouse (FIRE_RESIST)
COMSOL	Mesoscale: statistical methods, Continuum solid mechanics (micro) ; continuum thermodynamics; electrochemistry; continuum EM	www.comsol.com
CP2K	Electronic: quantum mechanical and Atomistic: ab-initio molecular dynamics and Quantum	www.cp2k.org

	Mechanics/Molecular Mechanics	
CRYSTAL MAKER	Electronic: quantum mechanical	www.crystalmaker.com
CTQMC	Electronic: many-body and semi-empirical or parametrised electronic models	inhouse (GOFAST)
CTS studio suite	continuum EM	www.cst.com/2010
DALTON	Electronic: quantum mechanical	www.dirac.chem.sdu.dk/daltonprogram.org/
DEFORM3D	Continuum mechanics (macro)	www.deform.com/products/deform-3d/
DEMON2K	Electronic: quantum mechanical	www.demon-software.com
DESSIS	Device modelling	www.iue.tuwien.ac.at/phd/klima/node8
DETCHEM	Continuum: Chemistry	www.detchem.com
DIFFRACMOD	Continuum EM	www.foservice.com/SOFTWARE/diffractmod
DGCA	Mesoscale: micromagnetics, file compression	inhouse (DYNAMAG)
DL_POLY	Electronic: quantum mechanical and device level	http://www.stfc.ac.uk/cse/25526.aspx
DMM	Mesoscale: micromagnetics This is a frequency domain technique rather a simulation code	In-house [DYNAMAG and MAGNONICS]
ELK	Electronic: quantum mechanical	www.elk.sourceforge.net
ETAOPT	Electronic: quantum mechanical	www.ise.fraunhofer.de/de/geschaeftsfelder-und-marktbereiche/alternative-photovoltaik-technologien/iii-v-epitaxie-solarzellen-und-bauelemente/simulation/etaopt
FDMAX	Continuum: Electomagnetics	
FEAP	Continuum solid mechanics (micro) and process	www.ce.berkeley.edu/feap
FEMAP	Commercial continuum solid: pre-processor	www.plm.automation.siemens.com
FEMME	Mesoscale: micromagnetics	www.suessco.com/simulations/solutions/femme-software
FIREBALL	Electronic: quantum mechanical	http://onlinelibrary.wiley.com/doi/10.1002/pssb.201147259/abstract;jsessionid=7E7A482F6EFD483AEB9979289EDEE0EE.d03t04)
FLAPW-FLEUR	Electronic: quantum mechanical, DFT	www.flapw.de
GARAND	Atomistic: statistical methods; drift diffusion	www.goldstandardsimulations.com/services/service-simulations/statistical-variability/atomistic-simulator

GAUSSIAN	Electronic: quantum mechanical and many-body and semi-empirical or parametrised electronic models and Atomistci Quantum Mechanics/Molecular Dynamics and Atomistic: statistical methods	www.gaussian.com
GPAW	Electronic: quantum mechanical	www.csc.fi/english/research/software/gpaw
GROMACS	Electronic: many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods, molecular dynamics	www.gromacs.org/About_Gromacs
GROMOS	Mesoscale: molecular dynamics	www.gromos.net
HYPERCHEM	Electronic: semi-empirical and ab-initio molecular orbital methods, as well as density functional theory Atomistic: molecular mechanics, molecular dynamics,	www.hyper.com
KMC-MD	Atomistic: statistical methods (Molecular Dynamics - kinetic Monte Carlo)	www.kintechlab.com/products/md-kmc
LAMMPS	Atomistic: statistical methods (molecular dynamics)	www.lammps.sandia.gov
LLG	Mesoscale: Micromagnetics	http://llgmicro.home.mindspring.com
Madrid/Konstanz code	Mesoscale: micromagnetics	Inhouse (FEMTOSPIN)
MAGPAR	Mesoscale: micromagnetics	www.magpar.net
MARC	Continuum mechancis (macro)	www.mscsoftware.com/Products/CAE-Tools/Marc.aspx
MATERIALS STUDIO	Electronic: many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods and Mesoscale: statistical methods	www.accelrys.com/products/materials-studio
MCGEN	Macro-scale: device modelling	Inhouse (SUPERLION)
MicroMagus	Mesoscale: micromagnetics	http://www.micromagus.de/
MSC.MARC/MENTAT	Macro-scale: Continuum solid mechanics (micro and macro); fluid dynamics; process	www.mscsoftware.com
MSINDO	Electronic: many-body and semi-empirical or parametrised electronic models	www.thch.uni-bonn.de
MUMAX	Meso-scale: micromagnetics	code.google.com/p/mumax
NAMD	Electronic: many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods	www.ks.uiuc.edu/Research/namd
NMAG	Mesoscale: micromagnetics	www.nmag.soton.ac.uk
NMTO	Electronic: many-body and semi-empirical or parametrised electronic models	www2.fkf.mpg.de/andersen
NXNastran	Continuum solid mechanics	http://www.plm.automation.siemens.com
OCTOPUS	Electronic: quantum mechanical in response of time dependent fields	www.tddft.org

OOMMF	Mesoscale: micromagnetics	www.ngs.ac.uk/use/applications/engineering/oommf
OpenKIM	Atomistic: interatomic potentials and simulations	www.openkim.org
OPENMX	Electronic: quantum mechanical	www.openmx-square.org
OPTILAYER	Continuum: EM	www.optilayer.com
OPTIWAVE	Continuum: EM	www.optiwave.com
PICMC (DSMC)	Atomistic: statistical methods	(ORAMA)
POM-POM TUBE	Macro-scale: fluid dynamics: polymer melt rheology This is a constitutive equation not a simulation package!	(MODIFY)
PWM	Mesoscale: micromagnetics	inhouse (DYNAMAG)
PWSIC	Electronic: quantum mechanical	Inhouse (ATHENA)
QUATRA/CELS	Atomistic: semi-classical drift-diffusion method and quantum kinetic model	inhouse (SMASH)
QLDFT	Electronic: quantum mechanical	physics.joacobs.university.de/theine/research/qldft/
QUANTUM ESPRESSO	Electronic: quantum mechanical and Atomistic: ab-initio molecular dynamics	www.quantum-espresso.org
QUIP	Electronic: quantum mechanical and Atomistic: ab-initio molecular dynamics and Quantum Mechanics/Molecular Mechanics	www.libatoms.org
RANDOMSPICE	Device modelling: statistical circuit simulator	www.goldstandardsimulations.com/products/randomspice
RETICOLO	Continuum: Electromagnetism	(NIM-NIL)
RIG-VM	Boltzmann transport equation solver, Direct Simulation Monte-Carlo and Particle in Cell plasma modelling for coating processes, optical modelling	http://www.ist.fraunhofer.de/en/services/simulation.html
RSPt	Electronic: many-body and semi-empirical or parametrised electronic models	www.fplmto-rspt.org
SE-MARGL	Mesoscale: micromagnetics This software for post-processing the data from micromagnetic simulations	www.magnonics.org/semargl/
SIESTA	Electronic: quantum mechanical and and many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods	www.nanotec.es/products/siesta.php
SPINPM	Mesoscale: micromagnetics	www.apl.aip.org/resource/1/applab/v96/i2/p022504_s1?view=refs
TIBERCAD	Electronic: many-body and semi-empirical or parametrised electronic models, continuum mechanics (micro)	www.tibercad.org/
TINKER	Electronic: many-body and semi-empirical or parametrised electronic models and Atomistic: statistical methods	www.dasher.wustl.edu/ffe/
TURBOMOLE	Electronic: quantum mechanical and quantum mechanical in response of time dependent fields	www.turbomole.com/

UppASD	Atomistic: statistical methods and Mesoscale: micromagnetics	Inhouse (MONAMI)
Uppsala code	Electronic: quantum mechanical in response of time dependent fields	Inhouse (FEMTOSPIN)
VASP	Electronic: quantum mechanical and Atomistic: ab-initio molecular dynamics and Quantum Mechanics/Molecular Mechanics	www.vasp.at
WANT	Electronic: quantum mechanical	(ATHENA)
WIEN2K	Electronic: quantum mechanical	www.wien2k.at
WISETEX	Continuum: solid and fluid mechanics	www.mtm.kuleuven.be/Onderzoek/Composites/software/wisetex
YORK code	Atomistic: statistical methods	Inhouse (FEMTOSPIN)

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This brochure is about modelling of materials, their properties and behaviour. It does not require prior knowledge of the subject. It is written for anybody interested. It contains no equations.

The brochure is to provide insight into the work of the modellers and help the reader to see the models as more than mere “black boxes”.

The models discussed span the complete materials field where important physics and chemistry can be very different. This is illustrated by modelling work carried out in the FP7 Industrial Technologies NMP Materials projects.

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