2.1.2 Report on the Workshop "Multiscale Approaches to Nanomechanics"

CECAM, Lyon (France)

5th-7th February 2007

SPONSORS

ESF Psi-k Programme
CECAM
ESF SimBioMa Programme
COST-P19 Action

ORGANIZERS

Ruben Perez
Universidad Autonoma de Madrid, Madrid, Spain

Karsten Reuter
Fritz-Haber-Institute, Berlin, Germany

http://www.cecam.fr/index.php?content=activities/pastWorkshops&action=details&wid=70

Summary

This meeting has focused on the application of computer simulations to the study of the microscopic aspects that determine the mechanical behavior of materials. This includes the structure and interaction of atomic-scale defects involved in macroscopic failure (crack tips, dislocation cores, grain boundaries, etc), mechanical and electronic transport properties of nanocontacts, and the interaction between nanoasperities (tips) and surfaces which is behind both the operation of scanning probes and the tribological contact between two materials. All these problems share an essentially multi-scale nature that requires a combined treatment of the different length (or time) scales: e.g. the breaking and formation of atomic bonds are dynamically coupled by long-range interactions (elasticity) to the macroscopic boundary conditions (deformation, load) imposed.

Nanomechanics describes the land where scanning probe experiments at the atomic and nanometer scale, the characterization of nanomaterials (e.g. nanotubes, nanocrystals and biomolecules) and computer simulations are currently meeting. This recently-born field spans both the methodological developments in the theoretical description of the different scales (from first-principles to continuum approaches) and the detailed experimental characterization achieved in the last few years, that provides a natural testing ground for those theoretical methodologies designed to bridge the length and time scales.

Following this perspective, the workshop has gathered 55 participants, including 25 invited speakers and session chairs, working in a broad range of problems and scientific disciplines. The event attracted a significant attention and 30 regular participants had to be selected among the 45 applications received in order to accommodate the meeting in the CECAM premises. The program was design to convey a balanced view of both the grand challenges in Nanomechanics and particularly promising methodological advancements. The 17 invited contributions (50 minutes, including 15 minutes discussion) were delivered by leading experts that provided an in-depth view of different theoretical and experimental approaches developed to address the mechanical and transport properties of systems of increasing size and complexity.The session chairs played a key complementary role, identifying strengths and weaknesses of the different particular approaches and stirring the discussion. The program included a lively poster session with 21 contributions, where the discussion extended well beyond the allocated time in the first evening of the meeting into the breaks in the following days.

The meeting has clearly shown the fundamental advances on the experimental side, based on the application of scanning probes. These detailed measurements, that challenged our current understanding and provide accurate quantitative data (even at the single defect level) to confront with the simulations, are the driving force for new theoretical developments. Two aspects emerge as key candidates for new approaches in order to bridge the length and time gap: the simulation under realistic conditions of the nucleation and mobility of point an extended defects, and the complex dynamics of the nanoasperities, the nanoscale objects that control the macroscopic properties of the mechanical contact between two materials.

Scientific Content and Discussion:Highlights

The program content and the abstracts of the different contributions can be found below. In the following we highlight some of the relevant ideas presented in the invited talks.

The three talks in the first day of the workshop, in a session chaired by Peter Gumbsch, addressed from both a theoretical and experimental perspective most of the relevant problems in the field. The first contribution, by Sidney Yip, provided a nice overview of how atomistic simulations can be used to study the nucleation of defects in an homogeneous material under a large strain deformation. This general paradigm was illustrated with applications to nanoindentation (discussing the competition between twinning and slip, and how to pass the yield criteria from atomistic to continuum simulations), dislocation loop emission (pointing out the problem of overdriving the system when using MD simulations) and chemomechanics (water attack on quartz). He ended with a particularly challenging technological problem that requires multi-scaling in both the space and time scales: understanding the time evolution of the shear modulus in cement. The talk by Erik van der Giessen showed that the limitations of both pure atomistic and continuum methodologies in order to predict the size dependence of plastic deformation can be overcome with the discrete dislocation plasticity (DDP) approach. He described the rules behind DDP simulations, showed their predictive power at size scales of tens of micrometers and smaller, and stressed the increasing importance of interfaces and boundaries (leading to hardening by pile-ups and strain gradients) when the dimensions of the sample are reduced. Finally, Joost Frenken described recent experiments on atomic-scale friction, where surprising regimes beyond the usual stick-slip behaviour have been found. These include superlubricity, and thermolubricity in layered solids, and the puzzling friction properties of water adsorbed on surfaces. Understanding these nanotribology experiments seems to require a detailed quantitative consideration of the mechanical response and the dynamics of the more mobile tip apex and the rest of the mechanical sensor as independent objects, that is beyond our current capabilities. The simple models that they have considered already questioned some of the basic assumptions in tribology regarding the microscopic channels and time scales for dissipation, and the definition of a microscopic friction coefficient. This talk promoted a lively discussion that extended into the poster session that closed the first day of the workshop.

The morning session in the second day, chaired by Alessandro de Vita, showed again the confrontation between the experimental challenges and some of the more sophisticated theoretical approaches. The session started with a presentation by Mike Payne on linear scaling ab initio methods. After discussing common features in most of these methods, (e.g. the expansion of the density matrix in terms of localized orbitals and a kernel, and the use of the idempotency to satisfy the orthogonality conditions), he focused on the ONETEP code, describing two key aspects of this implementation: (i) the use of a minimal basis of non-orthogonal generalized Wannier functions (NGWFs) adapted to the local environment , and (ii) the PSINC basis (real linear combination of plane waves) employed to span the NGWFs. He showed the accuracy and scalability of the method with different applications, including biological systems. Oscar Custance introduced the experimental perspective, presenting recent experiments with the atomic force microscope (AFM) operated in the dynamical mode that illustrated its capability to image, manipulate and even to chemically identifiy single atoms on surfaces. He also discussed the contribution of ab initio DFT calculations to the understanding of the imaging, manipulation and energy dissipation mechanisms at the atomic scale, and pointed out some of the problems, that are still waiting for more powerful ab initio or hybrid approaches. Alex Shluger addressed, from a theoretical perspective, the manipulation of surface atoms using either photons or an AFM. The first part of his contribution showed the need of an embedded cluster approach, where sophisticated quantum chemical methods can be integrated in order to describe light-induced selective desorption in oxide surfaces. Later, he described a virtual AFM method, where atomistic calculations, a Kinetic Montecarlo approach to bridge the time scale and a description of the electronics behind the operation of the microscope are integrated in order to provide a full account of the instrument response during the theoretical manipulation of an oxygen vacancy. Gabor Csanyi closed the morning session with a discussion of hybrid simulation schemes, where an empirical potential and a quantum mechanical model are combined into a single molecular dynamics simulation. He described different methodologies, based on the ”learning-on-the-fly” approach, to correct the potential in the relevant region in order to reproduce accurately the quantum mechanical forces, and discussed applications to brittle fracture (showing that reconstructions at the crack tip can lead to enhanced lattice trapping) and the properties of graphene ribbons.

Different contributions related to energy dissipation and friction were scheduled in the afternoon session, chaired by Ugo Valbusa. In the first talk, Jacqueline Krim presented three different experiments challenging our understanding of friction. She put particular emphasis in the complementarity of measurements taken with the quartz crystal microbalance and scanning probes (like the scanning tunneling microscope), pointing out the limitations of our current theories to describe the asperity contact point melting. Bo Persson was expected to provide the theoretical counterpart, with a discussion of contact mechanics and adhesion, but his talk had to be cancelled due to health problems. Michael Urbahk closed, in part, that gap with a model that linked the dynamics of formation and rupture of individual bonds with macroscopic friction properties. His approach, based on the relation between the equilibrium properties of the system and the mechanical forces measured under non-equilibrium conditions, extends its applicability to other relevant fields like the single-molecule pulling experiments designed to understand, from the unfolding process, the three-dimensional structure of proteins. The session ended with a detailed experimental discussion, by Nicolas Agrait, of the mechanical and transport properties of atomic chains formed in metal nanocontacts. The variation of those properties with the strain (including energy dissipation and inelastic currents related to the emission of single phonons) provided a very stringent test to our prospective multiscale approaches.

The morning session of the third day covered both strategies to bridge the time gap and to simulate and understand the implementation of pressure/load conditions, and was chaired by Giovanni Ciccotti. Laurent Pizzagalli presented the well-known ”nudged elastic band” approach for the determination of transition state energy barriers and discussed its application to the study of dislocation mobility. He focused on the calculation of the Peierls stress, pointing out the advantages and limitations of alternative methods based on either a direct calculation (where boundary conditions are the critical issue) or a Peierls-Nabarro approach based on the determination of the generalized stacking fault surface (problematic when the dislocation cores are narrow as in the case of Si). Eric van den Eijden discussed an alternative approach to the simulation of rare events: the string method. He started with a brief summary of transition state theory (that provides the basis for the method) and presented, with a simple two-dimensional example, the fundamentals of this algorithm to move curves over an energy landscape that is able to identify, in its zero- or finite-temperature versions, the minimum energy or minimum free energy paths. He concluded with a realistic application to the determination of the structure of a polymer chain in solvation. The experimental study of small-scale plasticity was the topic of the contribution by Andrew Minor. He showed how nanoindentation experiments performed inside a transmission electron microscopy provide access to a quantitative determination of the yield stress, through the simultaneous measurement of the imposed forces and the imaging of the induced deformations. These experiments, showing, for example, large yield stresses even in the presence of a large number of defects, challenge our understanding of the mechanical response of nanoscale objects. The session concluded with a theoretical talk by Carla Molteni on the simulation of pressure-induced structural transformations in semiconductor systems. She showed how to implement constant-pressure molecular dynamics simulations in both bulk and nanomaterials and discussed applications to the study of size-dependent properties in semiconductor nanocrystals under pressure.

The meeting ended with an afternoon session, chaired by Karsten Reuter, that illustrated the need of coarse-graining approaches to gain some understanding in complex systems. Alexis Baratoff discussed recent experiments where a small sinusoidal excitation of the cantilever leads to a regime with essentially vanishing friction. This novel regime can be understood with a simple extension of the classical friction models that takes into account the separation of the relevant time scales for the cantilever and the nanotip, the few atoms at the tip apex involved in the atomic-scale stick-slip processes. Berend Smit addressed the challenge of simulating the complexity of biological structures like cell membranes were purely atomistic approaches are not viable. Coarse-graining is the key tool to produce a manageable model that captures the repulsive (size-driven interactions) that control the packing and provides a good description of the phase diagram.

Conclusions and Perspectives

Nanotechnology, as an essentially cross-disciplinary field, still lacks the set of well-established concepts that characterize a mature discipline. This meeting has fulfilled the goal of gathering leading researchers from different communities (ab initio practitioners, molecular dynamics experts, material scientists, nanotribologists,) to share their expertise on the microscopic understanding of the mechanical properties of materials. The broad perspective delivered by the quite different topics covered by the invited speakers, and the lively discussions on particular conceptual or methodological aspects have contributed to the balanced view needed to identify common problems and interests. From this perspective, the meeting has contributed significantly to the definition of the core issues and challenges that should pervade the future development of Nanomechanics.

The main conclusions of the meeting can be summarized as follows:

- Although steady progress has been achieved in some particular aspects, this knowledge has not result in a fundamental, basic understanding of the mechanical response of materials. Some key ingredients have been identified (e.g. role of boundaries, defect mobility, see below) but we still lack a common framework that integrates all of them. The dispersion in methodological approaches and computational codes, devised in most cases for very specific applications, reflects this situation.
- Hybrid modelling, where the different length scales are dynamically coupled in a single simulation, is still a formidable task. Hierarchical multi-scale modelling –based on the optimal tools that we have for the different regimes (quantum mechanical, atomistic, quasi-continuum)– offers a viable alternative for many problems, where information can be extracted from one scale and passed to the next.
- Experiments are bridging the gap from the macroscopic to the nanoscale, providing relevant quantitative information (e.g. the yield stress for nucleation and response of a single defect, tip-sample forces for the diffusion of surface atoms) that can be directly used to validate the simulation approaches.
- The competition between nucleation and mobility of defects, and their interplay with boundaries (grains, interfaces,) and the chemical environment are key unifying microscopic concepts in the understanding of the mechanical response. Our current simulation approaches are still quite limited: they are affected by overdriving (due to the large gradients needed to create or move the defect) that contaminates the dynamical results, and they have severe limitations for considering all these processes at the same time.

- The rich phenomenology found in the mechanical contact between two materials (nanotribology) seems to be dominated by the interplay between the mechanical response and the dynamics of both small scale objects (tip apex, nanoasperities) and the macroscopic mechanical sensor considered as independent objects. The quantitative simulation of the resulting complex dynamics is still a theoretical challenge.

From the state of the art reflected in these conclusions, we should expect future developments in the field to follow these lines:

- Hybrid schemes, linking dynamically the different relevant length scales, are expected to play a key role in the final understanding of basic problems like brittle fracture. These developments will unifying concepts and well-tested, powerful codes that would stir further advancements in the field.
- There is an urgent need for new accurate and well-tested formulations to implement efficiently the elastic (load, pressure,..) boundary conditions and to extract information from atomistic simulations (e.g. yield stresses) into coarse-grained models, like Discrete Dislocation Plasticity and continuum approaches.
- A close collaboration between theory and experiment on well-defined problems (like tip-sample interaction in AFM) will make it possible to go beyond the mutual validation into real understanding.
- More systematic and efficient methods to explore rare events and identify minimum energy paths are needed in order to predict quantitatively the nucleation and mobility of defects. A real breakthrough in this field requires a joint effort of the ab initio and molecular dynamics communities.
- New methodological developments to break the time-scale gap (Accelerated Molecular Dynamics methods and efficient Kinetic MonteCarlo-like schemes) are needed in order to improve our fundamental understanding of nanotribology. The connections already identified between some equilibrium properties of nanoscale systems (easier to study theoretically) with the real non-equilibrium measurements performed in the experiments have to be further substantiated and expanded.

Program

Monday, February 5th

14:00 - 14:50	Registration	
14:50 - 15:00	Ruben Perez & Karsten Reuter	Welcome
		Chair: Peter Gumbsch
15:00 - 15:50	Sidney Yip	Nanoscale Characterizations of Shear Localization in Solids
15:50 - 16:40	Erik Van der Giessen	Discrete Dislocation Plasticity: Bridging a Gap
16:40 - 17:10	Coffee & Discussion	
17:10 - 18:00	Joost Frenken	Experiments on Atomic-Scale Friction: Superlubricity and Other Surprises
18:00 - 19:30	Poster Session & Buffet	

Tuesday, February 6th

		Chair: Alessandro de Vita
9:00 - 9:50	Mike Payne	The Linear Scaling Density Functional Theory Code ONETEP
9:50 - 10:40	Oscar Custance	Dynamic Force Microscopy: Imaging Contrast, Manipulation and Chemical Identification of Individual Atoms
10:40 - 11:20	Coffee & Discussion	
11:20 - 12:10	Alex Shluger	Manipulating Surface Atoms using Photons and AFM
12:10 - 13:00	Gabor Csanyi	Hybrid schemes for Atomistic Modelling
13:00 - 14:30	Lunch	
		Chair: Ugo Valbusa
14:30 - 15:20	Jacqueline Krim	Viewing a Moving Contact: A Scanning Probe and Quartz Crystal Microbalance Study of Sliding Friction and Melting at Single Asperity Contacts
15:20 - 16:10	Bo Persson	Contact Mechanics and Adhesin
16:10 - 16:40	Coffee & Discussion	
16:40 - 17:30	Michael Urbakh	Dynamical Rupture of Molecular Bonds: From Single Molecular Studies to Nanomanipulation and Friction
17:30 - 18:20	Nicolas Agrait	Mechanical Properties and Dynamics of Suspended Atomic Chains
19:30	Conference Dinner	

Wednesday, February 7th

		Chair: Giovanni Ciccotti
9:00 - 9:50	Laurent Pizzagalli	Determination of Dislocation Mobility from Transition States Searching Technique
9:50 - 10:40	Andy Minor	Direct Observation and Measurement of Small-Scale Plasticity Phenomena through in situ TEM Nanoindentation and Compression Tests.
10:40 - 11:20	Coffee & Discussion	
11:20 - 12:10	Eric Van den Eijden	String Method to Find the Pathways of Rare Events.
12:10- 13:00	Carla Molteni	Pressure-Induced Structural Transformations in Semiconductor Systems
13:00 - 14:30	Lunch	
		Chair: Karsten Reuter
14:30 - 15:20	Alexis Baratoff	A Novel Mechanism for the Efficient Reduction of Atomic-Scale Friction
15:20 - 16:10	Berend Smit	Simulating Mesoscopic Models of Biological Membranes
16:10 - 16:30	Closing Remarks	

ABSTRACTS OF INVITED TALKS

Nanoscale Characterizations of Shear Localization in Solids

Ting Zhu[1], Ju Li[2], Shigenobu Ogata[3], Jingpeng Chang[4], Krystyn Van Vliet[5], Subra Suresh[5] and Sidney Yip[4,5,*]

[1] *Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332*

[2] *Department of Materials Science and Engineering, Ohio State University, Columbus, OH 43210-1178*

[3] *Department of Mechanical Engineering, Osaka University, Osaka 565-0871, Japan*

[4] *Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139-4307 (USA)*

[5] *Depaqrtment of Materials Science and Engineering, Massqchusetts Institute of Technology, Cambridge, MA 02139=4307 (USA)*

The phenomenon of defect nucleation in a crystal lattice is fundamental to our understanding of materials strength and deformation. Through atomistic simulations we examine how a dislocation slip or a deformation twin can form as a result of shear localization in response to an imposed stress field. Three scenarios will be described to illustrate our attempts to formulate dynamical measures of such processes at the nanoscale. In nanoindentation of a single-crystal thin film we show a local stiffness criterion can be developed to account for the displacement bursts associated with dislocation nucleation and multiplication. By subjecting a perfect crystal to affine shear we find the formation of a deformation twin evolves as an instability of a non-linear wave. To model the advancement of a crack front we use reaction pathway sampling to determine the saddle-point configuration, which leads to the bowing out of a dislocation loop in the case of a ductile metal (Cu), and the nucleation and propagation of double kinks in the case of a brittle semiconductor (Si). Scrutiny of these results, based thus far on empirical interatomic potentials, by density functional theory methods would be illuminating.

Discrete Dislocation Plasticity: Bridging a Gap

Erik van der Giessen

Micromechanics of Materials Group. Department of Applied Physics. University of Groningen.
9747 AG Groningen, The Netherlands

Although much is known about the atomic structure of dislocations, the link to what we observe on larger scales as plastic deformation is still largely elusive. A key reason is the large separation of scales, for which the study of individual dislocations remained in the realm of physics while plasticity was an engineering topic. During the last decade however, the gap between these started to be filled by discrete dislocation plasticity. This is an approach where the atoms are averaged-out and treated as an elastic continuum, while the dislocations are regarded as discrete entities. Discrete dislocation computations are useful in the range of size scales where there are too many dislocations to be treated atomistically but not enough to be averaged-out to continuum plasticity. This transition happens to lie around a micrometer, a length scale that is typical in current MEMS applications. Moreover this is roughly the sizescale at which numerous plasticity phenomena are taking place that exhibit size effects inaccessible by standard continuum theories.

In view of the other sessions in this workshop, I will supplement the exposition of the approach with some examples concerning indentation, contact and friction.

Experiments on Atomic-Scale Friction: Superlubricity and Other Surprises

Joost W.M. Frenken

Kamerlingh Onnes Laboratory, Leiden University, The Netherlands,
frenken@physics.leidenuniv.nl, www.physics.leidenuniv.nl/sections/cm/ip

This talk will provide a brief summary of Friction-Force Microscopy (FFM) experiments, in which a sharp tip is moved over a flat substrate with atomic-scale precision, while the lateral forces are recorded with a sensitivity down to the low picoNewton regime. Whereas the first measurements in this field have demonstrated a variety of atomic-scale lateral force patterns, related to stick-slip motion of the tip in the periodic, two-dimensional surface of the interaction potential between the tip and the substrate, recent experiments and model calculations are revealing important new ingredients. In particular, I will address lattice mismatch effects that can lead to superb slipperiness (*'superlubricity'*), thermal effects that can dramatically lower friction (*'thermolubricity'*) and multiple-mass-multiple-spring effects that can lead to quite unexpected sliding dynamics [3].

[1] M. Dienwiebel *et al.*, *Phys.Rev.Lett.* **92**, 126101 (2004); ibid. *Surf.Sci.* **576**, 197 (2005); G.S. Verhoeven *et al.*, *Phys.Rev. B* **70**, 165418 (2004).

[2] S.Yu. Kryolov *et al.*, *Phys.Rev. E* **71**, 065101 (2005).

[3] S.Yu. Krylov *et al.*, *Phys.Rev.Lett.* **97**, 166103 (2006).

The Linear Scaling Density Functional Theory Code ONETEP

M.C. Payne, P.D. Haynes, C.K. Skylaris and A. Mostofi

University of Cambridge, United Kingdom

ONETEP is a density functional theory code that offers the same accuracy as state of the art plane wave approaches but offers efficient and robust convergence to the electronic groundstate in a computational time that scales linearly with the number of atoms in the system. This code allows first principles calculations to be performed for systems containing thousands of atoms at very modest cost both in terms of computational resources and money. The ability to perform calculations for so many atoms provides much greater flexibility in the choice of quantum region in QM/MM or hybrid simulation schemes. ONETEP allows one to choose the range of the density matrix and this can be used to rigorously assess the errors introduced by truncating the QM region in hybrid simulations.

Dynamic Force Microscopy: Imaging Contrast, Manipulation and Chemical Identification of Individual Atoms

Oscar Custance

Graduate School of Engineering, Osaka University, Japan

Dynamic force microscopy is a particularly promising technique in nanoscience. This scanning probe method makes it possible, for instance, to image both conducting and insulating surfaces with true atomic resolution [1], to manipulate atoms at surfaces even under room temperature conditions [2], or to characterize the chemical composition of a surface at atomic scale [3]. Most of these capabilities are closely related to the nanomechanical properties of the surface under study and the tip-apex probing it, linked though the short-range chemical interaction forces between the tip-surface closest atoms. The ability to quantify very precisely these chemical forces [4-6] makes DFM a suitable and challenging method for the combination of experiments and theoretical approaches on nanomechanics. In this contribution we will present some of the latest mayor achievements in DFM, in which the combination of experiments and first-principles calculations has shown to be particularly useful to understand the complicated processes observed [3, 4-7].

[1] Morita, S., Wiesendanger, R. & Meyer, E. *Noncontact Atomic Force Microscopy.* NanoScience and Technology (Springer-Verlag, Berlin, 2002)

[2] Y. Sugimoto, M. Abe, S. Hirayama, N. Oyabu, O. Custance and S. Morita, *Nature Materials* **4**, 156 (2005)

[3] Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Perez, S. Morita, and O. Custance (accepted)

[4] M. A. Lantz, H. J. Hug, R. Hoffmann, P. J. A. van Schendel, P. Kappenberger, S. Martin, A. Baratoff, H.-J. Güntherodt, *Science* **291**, 2580 (2001)

[5] M. Abe, Y. Sugimoto, O. Custance, and S. Morita, *Appl. Phys. Lett.* **87**, 173503 (2005)

[6] N. Oyabu, P. Pou, Y. Sugimoto, P. Jelinek, M. Abe, S. Morita, R. Perez and O. Custance *Phys. Rev. Lett.* **96**, 106101 (2006)

[7] Y. Sugimoto, P. Pou, O. Custance, P. Jelinek, S. Morita, R. Perez and M. Abe, *Phys. Rev. B* **73**, 205329 (2006)

Manipulating Surface Atoms using Photons and AFM

Alexander Shluger

Department of Physics and Astronomy, University College London, Gower St., London WC1E6BT, UK

I will discuss the results of some of our studies of atomic scale contacts between oxide nanoclusters and surfaces using different levels of multi-scale modelling. First, I will focus on applying an embedded cluster technique to study the structure, electronic properties and photo-induced modification of MgO and CaO powders. A variety of structural features will be considered that can be found on the surface of nanoclusters as well as at interfaces between nanocrystallites buried inside the powder. I will then focus on photo-induced desorption of hyper-thermal O, Mg (Ca) atoms from the MgO and CaO surfaces and will show that the yield, electronic state, and velocity distributions of desorbed atoms can be controlled due to preferential excitation of surface excitons. MgO nanoclusters are also used as model tips for simulating non-contact Atomic Force Microscopy imaging of ionic surfaces and manipulation of surface atoms and adsorbates. In this case combining both different length- and time-scales is important. Our simulations predict that controlled manipulation of a charged surface O vacancy and adsorbed atoms, such as Pd, on the MgO (001) surfaces can be achieved via the reduction of diffusion barriers by the tip electrostatic potential, which facilitates thermal diffusion. Modelling of the full manipulation process involves much slower tip oscillations and even slower response of the AFM electronics.

Hybrid schemes for Atomistic Modelling

Gabor Csanyi

University of Cambridge, United Kingdom

I will present updates on our going efforts in hybrid atomistic modelling, whereby an empirical potential and a quantum mechanical model are combined into a single molecular dynamics simulation. Fundamental limitations of this approach will be discussed, along with several ways of combining the two models. Practical examples include fracture, defect energetics and biomolecular modelling.

Viewing a Moving Contact: A Scanning Probe and Quartz Crystal Microbalance Study of Sliding Friction and Melting at Single Asperity Contacts

J. Krim

Department of Physics, Box 8202, North Carolina State University,Raleigh, NC 27695-8202

Energy transfer plays an important role in many surface processes such as surface diffusion, vibrational relaxation and sliding friction in adsorbed molecules. The Quartz Crystal Microbalance has in recent years been employed to reveal much fundamental information on the phononic and electronic energy dissipation mechanisms associated with the sliding of atomically thin films along surfaces, a phenomenon closely related to the spreading diffusion of a film on its substrate.[1] While in quantitative agreement with theory and computer simulation, the QCM data have not been cross-referenced to scanning probe measurements of sliding friction and diffusive behavior of atoms along surfaces. We have thus combined a Scannning Tunneling Microscope and QCM to allow direct imaging of films adsorbed on the QCM electrode under both stationary and oscillating conditions.[2] The results of these studies will be described, along with a discussion of whether our current knowledge of the fundamentals of friction is sufficient to enable prediction of asperity contact point melting.

[1] *STM, QCM and the Windshield Wiper Effect: A Joint Theoretical-Experimental Study of Adsorbate Mobility and Lubrication at High Sliding Rates.* M. Abdelmaksoud, S. M. Lee, C. W. Padgett"D. Inving, D.W. Brenner, and J. Krim, Langmuir, in press

[2] *Observation of tribo-induced melting of an asperity contact with STM-QCM,* S. M. Lee, D. L. Irving, C. W. Padgett, D.W. Brenner, and J. Krim, Phys. Rev. Lett, submitted

Contact Mechanics and Adhesion

B.N.J. Persson,

IFF, Research Center Jülich, Germany

Adhesion and friction becomes more important when the lateral size of objects decreases. This is due to the increased surface to volume ratio. At the micro and nanoscale the gravitational interaction is usually negligible compared to the van der Waals interaction and electrostatic interactions, or forces due to the formation of small (nanometer) capillary bridges. Problems related to adhesion and friction (and wear) are the most severe problems to be overcomed in the development of many useful micro or nanoscale mechanical systems, e.g., micromotors. In this presentation I will describe a new theory of contact mechanics for solids with randomly rough surfaces. I consider the elastic contact between solids both without and with adhesion. As an illustration I will discuss in detail biological adhesion systems used for locomotion, and show how Natural selection in some cases has optimized the adhesive systems from the (macroscopic) size of the adhesion pads (typically of order _ 1 mm) to the nanoscale. As a second application of the theory I will briefly describe rubber friction on rough substrates.

Dynamical Rupture of Molecular Bonds: From Single Molecular Studies to Nanomanipulation and Friction

Michael Urbakh

School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel.

Single molecular pulling experiments using atomic-force microscopes or laser tweezers are widely used to probe rare molecular events, such as rupture of molecular bonds and protein unfolding. In order to explore the results of these experiments and to reveal a molecular scale energy landscapes, one has to establish relationships between equilibrium properties of the nanoscale systems and the mechanical forces measured under non-equilibrium conditions. Here we introduce a new approach to describe unbinding processes measured by dynamical force spectroscopy experiments that predicts a distribution of rupture forces, and dependences of mean rupture forces and variance on the pulling velocity. It was shown to reproduce the results of simulations without using adjustable parameters. Our analysis predicts that the mean force at rupture is a nonlinear function of the logarithm of the pulling velocity. We show that understanding unbinding processes on the single-molecule level opens new ways for manipulation of individual molecules at surfaces.

We propose a microscopic model that establishes a relationship between the dynamics of formation and rupture of individual bonds and macroscopic frictional phenomena. In particular, the stick-slip regime of motion is shown to correspond to a cooperative rupture of the bonds.

Mechanical Properties and Dynamics of Suspended Atomic Chains

Nicolás Agraït

Low Temperature Laboratory. Universidad Autónoma de Madrid (Spain)

Freely suspended atomic chains form spontaneously during the final stage of rupture of a metal contact of certain metals (Au, Pt, Ir). These nanostructures are very attractive because being so simple in structure they are amenable to detailed theoretical calculations of structure and transport using state-of-the-art ab initio methods, allowing for direct comparison between experiments and theory. Electronic transport and mechanical properties have been studied experimentally and theoretically in some detail. In this talk I will review the mechanical and vibrational properties of atomic chains and present new recent experimental results on the interatomic interaction dynamics in the chains.

Determination of Dislocation Mobility from Transition States Searching Technique

L. Pizzagalli, P. Beauchamp, A. Pedersen, A. Arnaldson, and H. Jonsson

CNRS, France

Dislocations are extended defects present in almost all materials that govern the mechanical response in the plastic regime. Their properties and behaviors under stress are then important to characterize for a better understanding of mechanical properties of materials. Recently, numerous works have been devoted to core dislocations modeling using first principles methods. This especially concerned stability and structure. For a complete understanding of the plastic properties of materials, quantities related to dislocations mobility (critical stress, kinks formation,...) have to be determined as well. However, due to the technical limitations associated with conventional atomistic methods, less informations are available.

Here, we present the results of first principles and potentials simulations on dislocation mobility in semiconductors, using transition states searching technique such as Nudged Elastic Band. In a first part, we show how this technique can be used to determine the Peierls stress of perfect dislocations in silicon, how pressure would affect this value, and how a dislocation shape changes during its displacement. In a second part, we discuss the mobility of dislocations through kinks formation/migration.

Direct Observation and Measurement of Small-Scale Plasticity Phenomena through *in situ* TEM Nanoindentation and Compression Tests

A. M. Minor

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA

The technique of quantitative *in situ* nanoindentation in a transmission electron microscope (TEM) allows for the simultaneous measurement of the imposed forces and imaging of the initial stages of plasticity in materials. Individual yield events in a material can be directly correlated with the stress required to initiate specific deformation events. This talk will demonstrate this capability from results on the in situ nanoindentation of Al thin films and in situ compression of nanostructured Ni and Al pillars. In the Al thin films we have observed that high stresses are achieved in the Al thin films even in the presence of significant defects. In situ compression experiments on single crystal Ni and Al pillar structures directly demonstrate the phenomenon of source-limited deformation, where plasticity is derived from single or very few active slip systems in samples with sub-micron dimensions. These results will be discussed in terms of current and future computational efforts to model and predict similar deformation phenomena.

String Method for the Study of Rare Events

Eric Van den Eijden

Courant Institute of Mathematical Sciences, New York, USA

The string method is a simple and efficient technique for computing accurately minimum energy paths (MEPs) and minimum free energy paths (MFEPs). I will introduce the theoretical background behind the method, discuss its algorithmic details and illustrate it via examples.

Pressure-Induced Structural Transformation in Semiconductor Systems

Carla Molteni

Kings College London, United Kingdom

Pressure can be used as a tool for inducing structural transformations between distinct crystalline and/or amorphous structures. Polymorfism and polyamorphism phenomena can be studied by means of constant-pressure molecular simulations in both bulk- and nano-materials. In particular semiconductor nano-crystals under pressure exhibit a range of interesting size-dependent properties, which need to be dealt with specific techniques for non-periodic systems. Still constant pressure molecular dynamics simulations for structural phase transformations suffer from shortcomings due to the limited accessible time-scale; while solutions have been proposed for periodic bulk systems, methods for non-periodic systems need to be explored. Results and ideas for cadmium selenide and silicon bulk- and nano-crystals will be presented.

A Novel Mechanism for the Efficient Reduction of Atomic-Scale Friction

S. Maier, A. Socoliuc, A. Baratoff, E. Gnecco, E. Meyer

National Center of Competence in Research (NCCR) on Nanoscale Science, Institute of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The transition from atomic-scale stick-slip to continuous sliding with essentially vanishing friction predicted by the Prandtl-Tomlinson model has clearly been observed for a sharp atomic force microscope tip slowly scanned in contact with a cleaved NaCl crystal in UHV [1]. A similar transition under the same conditions has recently been achieved upon excitation of a flexural mode of the cantilever bearing the tip [2]. In contrast to the previously observed or predicted reduction of friction in the presence of driven oscillations [3], the effect is not associated with a time-average increase of the tip-sample distance.

We consider in detail a dynamic extension of the model introduced earlier [1]. On one hand, the observed dependence of the lateral force along the scan direction implies an oscillating corrugation potential experienced by the tip. On the other hand, the observed low contact stiffness suggests that atomic-scale stick-slip mainly involves elastic energy stored and released by a few atoms around the tip apex. Atomistic support this conjecture. These *a priori* unexpected results lead to a model which accounts well for the new measurements in the presence of perpendicular sinusoidal excitation [2]. In view of the separation of the relevant time scales for the cantilever and the "nanotip", the observed reduction of friction can be explained in terms of parameters extracted from quasistatic measurements alone. Deviations from adiabatic following cause a residual viscous-like friction which is independent of damping and to a concomitant energy loss. Remarkably, the total loss, including the contribution from the periodic actuation, can be considerably smaller than in the absence of the latter. Simple physically motivated approximations can explain our numerical results

[1] A. Socoliuc, R. Bennewitz, E. Gnecco, E. Meyer, Phys. Rev. Lett. 92, 134401 (2004)

[2] A. Socoliuc, E. Gnecco, S. Maier, O. Pfeiffer, A. Baratoff, R. Bennewitz, E. Meyer, Science 313, 307 (2006)

[3] M. Urbakh, J. Klafter, D. Gourdon. J. Israelachvili, Nature 430, 525 (2004)

[4] S. Maier, PhD Thesis, University of Basel (2007)

Simulating Mesoscopic Models of Biological Membranes

Berend Smit, Maddalena Venturoli and Frederic de Meyer

CECAM, Lyon, France

In this presentation a mesoscopic model of a biological membrane is presented. We show that this model can correctly describe the phase behaviour of a phospholipid membrane. We investigated the phase behavior of double-tail lipids, as a function of temperature, headgroup interaction and tail length. At low values of the head-head repulsion parameter the bilayer undergoes with increasing temperature the transitions from the subgel phase via the flat gel phase to the fluid phase. We find that the rippled structure occurs if the headgroups are sufficiently surrounded by water. The anomalous swelling, observed at the transition, is not directly related to the rippled phase, but a consequence of conformational changes of the tails. This model is subsequently used to study the effect of alcohol and transmembrane peptides on the structure of the membrane.

[1] Kranenburg, M.; Laforge, C.; Smit, B. Physical Chemistry Chemical Physics 2004, 6, 4531.

[2] Kranenburg, M.; Vlaar, M.; Smit, B. Biophysical Journal 2004, 87, 1596.

[3] Venturoli, M.; Smit, B.; Sperotto, M. M. Biophysical Journal 2005, 88, 1778–1798.

[4] Kranenburg, M.; Smit, B. J. Phys. Chem. B 2005, 109, 6553.

[5] Venturoli, M.; Sperotto, M. M.; Kranenburg, M.; Smit, B. Physics Reports 2006, 437, 1 – 54.

POSTER LIST and ABSTRACTS

1. Metadynamics simulations of phase transitions in solids
   by **Jörg Behler**, Michele Parrinello

2. An efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer Molecular Dynamics
by **Thomas Kühne**, Matthias Krack

3. Mechanical testing of nanocrystalline ceramics: massively parallel molecular dynamics simulations
by **Izabela Szlufarska**, Yifei Mo

4. Modelling strategies for ferritic steels
by **Maria Samaras**

5. Accurate periodic calculations using large Gaussian basis sets
by **Matthias Krack**

6. Tribological properties of adsorbed Xe-layers on Cu(111) surface
by **Maria Clelia Righi**

7. Understanding the cleavage of diamond from the bond breaking
by **Pablo Pou**, Rubén Pérez and Peter Gumbsch

8. Towards the symthesis of fullerene: triazafullerene adsorption on noble metal close packed surfaces
by **Giulio Biddau**, M. Basanta, J. Ortega, R. Pérez, G. Otero, B. Gómez-Lor, J.A. Martín Gago

9. First-principles study of the cubic-SiC(100) - 4x2 surface
by **Daniel Gonzalez**, D. González , P. Jelínek , J. Ortega

10. Density functional embedding for molecular systems
by **Marcella Iannuzzi**

11. Enhanced chemical reactivity of gold nanowires
by **Pavel Jelinek**, Rubén Pérez , Jose Ortega and Fernando Flores

12. Interstitials in FeCr studied by Density Functional Theory
by **Peter Klaver**, P. Olsson, M. W. Finnis

13. Hydrogen damage in metals: Constrained molecular dynamics and Monte Carlo simulations of superabundant vacancies
by **Döme Tanguy**, E. Vamvakopoulos

14. Study of In adsorption on a In-rich 2(2x4) InGaAs surface on GaAs(001)
by **Rita Magri**, Marcello Rosini

15. Effects of impurities on cohesion at $\Sigma5(210)$ grain boundary of magnetic metals
by **Elwira Wachowicz**, T.Ossowski and A. Kiejna

16. From individual defects to microstructures
by **Fabrizio Cleri**

17. Computational tools for modeling and simulation of nanoscale systems
by **Reinier Akkermans**
18. Metal adhesion at oxide ceramic interfaces
by **Carmen Muñoz**, J.I. Beltrán, S. Gallego and M.C. Muñoz
19. Relaxation of semiconductor interfaces by molecular dynamics using enhanced bond order potentials
by **Kurt Scheerschmidt**, Volker Kuhlmann
20. Multiscale hybrid simulations of brittle fracture
by **James Kermode**, Gabor Csanyi, A. De Vita, M.C. Payne
21. A cohesive zone model for stress corrosion cracking in ceramic polycrystals
by **Rafael Estevez**, M. Romero de la Osa, C. Olagnon, J. Chevalier, C. Tallaron, L. Vignoud

Metadynamics simulations of phase transitions in solids

Jörg Behler, Michele Parrinello

ETH Zurich, Switzerland

The chemical and physical properties of a solid are determined by its crystal structure, which depends on the temperature and pressure in the system. Often, the experimental determination of the crystal structure is very difficult or even impossible under extreme conditions, which are present e.g. in the interior of the earth and other planets. Therefore, in recent years the theoretical prediction of crystal structures has become a valuable tool to investigate solids under these conditions. The stability of a structure is given by its Gibbs free energy, and the hypersurface of the Gibbs free energy can be systematically mapped by the recently developed metadynamics approach. In this method the Gibbs free energy is represented as a function of the unit cell parameters, which are modified by introducing Gaussian potentials. This requires the calculation of the stress tensor for many different unit cells by molecular dynamics (MD) simulations. If no fast and reliable potentials are available the only way to perform the MD simulations is to use potentials obtained directly from Density-Functional Theory (DFT), which for metadynamics is computationally too demanding even for systems of moderate size. In the present work we develop and employ a new type of Neural Network (NN) potential to represent the high-dimensional DFT potential-energy surface (PES) as a function of all atomic coordinates in the crystal. Tests show that an accurate fit can be obtained that correctly describes all known crystal structures of silicon. This NN potential is applied to metadynamics simulations of pressure-induced phase transitions in bulk silicon. We obtain phase transitions in good agreement with density-functional calculations and experiment.

An Efficient and Accurate Car-Parrinello-like Approach to Born-Oppenheimer Molecular Dynamics

Thomas Kühne, Matthias Krack

ETH Zürich, Switzerland

We present a new method to accelerate density functional theory-based ab-initio molecular dynamics simulations. In the spirit of the Car-Parrinello approach, the method circumvents the need to perform fully self-consistent electronic structure calculations. However, in contrast to the original scheme, large integration time steps can be used. To achieve this, we propagate the electronic degrees of freedom in terms of the contra-covariant density matrix in a nearly time-reversible manner by applying the always stable predictor-corrector method. The corrector consists of a single preconditioned minimization step using the idempotency conserving orbital transformation method. In this way sizable minimization steps can be taken, which guarantees that the propagation is performed within a small skin very close to its instantaneous ground state. Although the applied non-self-consistent energy functional is not variational, the energies thus calculated are a strict upper bound. Deviations from the Born-Oppenheimer surface are small and, more importantly constant, which implies that energy differences are portrayed with great accuracy. In spite of these excellent properties the incomplete energy minimization and the use of a non-symplectic integrator for the electronic degrees of freedom induces a small dissipative drift. Inspired by ideas of Krajewski and Parrinello we show how this can be rigorously corrected using a properly modified Langevin equation, which leads to correct sampling of the Boltzmann distribution. Furthermore the friction term is so small that the dynamics is also properly reproduced. The method works well irrespective of system type and band gap, so it is very efficient even in simulating large metallic systems. We implemented these ideas in the mixed Gaussian Plane Wave (GPW) code Quickstep which is part of the publicly available suite of programs CP2K. Using this code we performed extensive tests on liquid semiconductors showing that the accuracy can be maintained throughout. The gain in efficiency ranges from one to two orders of magintude depending on the system.

[1] R. Car and M. Parrinello, Phys. Rev. Lett. 55, 2471, (1985).

[2] J. Kolafa, J. Comput. Chem. 25, 335 (2004).

[3] J. VandeVondele and J. Hutter, J. Chem. Phys. 118, 4365 (2003).

[4] F. R. Krajewski and M. Parrinello, Phys. Rev. B 73, 041105(R), (2006).

[5] G. Lippert, J. Hutter and M. Parrinello, Mol. Phys. 92, 477 (1997).

[6] J. VandeVondele et al., Comp. Phys. Comm. 167, 103 (2005).

[7] http://cp2k.berlios.de/

Mechanical testing of nanocrystalline ceramics: massively parallel molecular dynamics simulations

Izabela Szlufarska, Yifei Mo

University of Wisconsin - Madison, United States

Atomistic mechanisms underlying the mechanical response of nanocrystalline ceramic thin films have been studied by multimillion-atom molecular dynamics simulations on parallel computers. The increased volume fraction of highly disordered intergranular films as compared to nanometals manifests itself in new deformation mechanisms. Our nanoindentation studies of nanocrystalline silicon carbide provide a scenario for the interplay between grain rotation, corporate grain motion, sliding at grain boundaries and integranular deformation to produce a rich and unique load-displacement response. We predict a crossover from continuous corporate grain response to discrete inter-grain plasticity at a critical depth that is a fraction of the grain size. We have also studied simulated the tensile and shear testing and described changes in the mechanical response resulting from the reduction of a grain size. Understanding of the fundamental phenomena that govern mechanical properties is crucial for design and fabrication of nanocrystalline materials with enhanced mechanical properties.

Modelling Strategies for Ferritic steels

Maria Samaras

Paul Scherrer Instititute, Switzerland

The safe and reliable performance of fusion and fission plants is dependent on the choice of suitable materials and assessment of long-term materials. These materials are degraded by their exposure to high temperatures, irradiation and a corrosive environment, therefore it is necessary to address the issue of long term damage evolution of materials under service exposure in advanced plants. The life-time assessments of these materials requires an understanding of the related physical phenomena on a range of scales from the microscopic level of single defect damage effects all the way up to macroscopic effects. Therefore it is necessary to have an understanding of the mechanisms at play at many different time and length scales. Computer modelling is expected will complement experimental work to enhance and speed up the assessments of the expected life-time of materials subjected to reactor conditions with the formulation of credible predictive computational models. These models must be developed with the verification of experiment, to accurately describe materials phenomena and to allow for extrapolation to longer time frames. In this poster the multiscale modelling strategies undertaken to study ferritic steels are presented. Within this frame work the influence of magnetism on the ferritic system and experimental validation of magnetic ab initio calculations using XMCD and XAFS are presented

Accurate Periodic Calculations Using Large Gaussian Basis Sets

Matthias Krack

Computational Science, ETH Zurich, via G. Buffi 13, 6900 Lugano, Switzerland

Condensed phase calculations using Gaussian basis sets for liquid and crystalline systems are presented. The calculation were performed with the QUICKSTEP code [1, 2]. QUICKSTEP is an implementation of the Gaussian and plane waves (GPW) method [3] based on the Kohn-Sham formulation of density functional theory. The hybrid scheme employed by QUICKSTEP uses a mixed basis set approach combining Gaussian functions and plane waves in order to exploit the advantages of both basis set types. Gaussian basis sets and pseudo potentials optimized for the use with QUICKSTEP are presented to show its accuracy [4]. The computational efficiency of QUICKSTEP allows to use large Gaussian basis sets including functions of high angular momentum and accurate pseudo potentials for systems up to several thousand atoms. The results of benchmark runs for water are presented to show the efficiency and scalability of QUICKSTEP. Moreover, the Gaussian augmented plane waves (GAPW) scheme [5] allows to perform all-electron calculations [6, 7] or to deal with very hard (i.e. accurate) pseudo potentials which are e.g. mandatory for systems containing first-row transition metals. Results of periodic all-electron and pseudo potential calculations for bulk pyrite (FeS2) are compared with other methods.

The QUICKSTEP code is part of the freely available program package CP2K (http://cp2k.berlios.de).

Acknowledgments

This work was partially supported by the DEISA Extreme Computing Initiative.

[1] M. Krack and M. Parrinello, QUICKSTEP*: Make the atoms dance*, volume 25 of *NIC Series*, NIC-Directors, 2004.

[2] J. VandeVondele et al., Comput. Phys. Commun. **167**, 103 (2005).

[3] G. Lippert, J. Hutter, and M. Parrinello, Mol. Phys. **92**, 477 (1997).

[4] M. Krack, Theor. Chem. Acc. **114**, 145 (2005).

[5] G. Lippert, J. Hutter, and M. Parrinello, Theor. Chem. Acc. **103**, 124 (1999).

[6] M. Krack and M. Parrinello, Phys. Chem. Chem. Phys. **2**, 2105 (2000).

[7] M. Iannuzzi, T. Chassaing, T.Wallman, and J. Hutter, Chimia **59**, 499 (2005).

Tribological properties of adsorbed Xe-layers on Cu(111) surface

M.C. Righi[1], L.R. Maurichi[1], M. Ferrario[1], A. Vanossi[1] and Erio Tosatti[2]

[1] *CNR-INFM National Research Center S3 and Department of Physics, University of Modena and Reggio Emilia, Via Campi 213/A, 41100 Modena, Italy*

[2] *International School for Advanced Studies (SISSA) and INFM Democritos National Simulation Center, Via Beirut 2, I-34014 Trieste, Italy International Centre for Theoretical Physics (ICTP), P.O.Box 586, I-34014 Trieste, Italy*

Progress in the ability of understanding tribological properties in adsorbed film systems is of paramount importance to unravel fundamental issues in the emerging field of nanoscale science and technology. Many extensive studies have used a quartz-crystal microbalance (QCM) to measure the friction between adsorbed layers and crystalline substrates. In this work, we report a theoretical investigation of the tribological behavior for solid Xenon monolayers physisorbed on the Cu(111) surface; this sliding interface has been recently investigated experimentally by Coffey and Krim [1]. In order to get a reliable description of the adsorbate/substrate interaction, we evaluate the potential energy landscape experienced by a Xe atom physisorbed on the Cu(111) surface by ab initio calculations. The static frictional properties are analyzed in details as a function of system temperature, presence of interlayer defects, load and the connected change of anticorrugation. Contrary to the QCM experimental results, we find that, due to perfect interface commensurability, the (full monolayer) system exhibits strong pinning. However, the numerical simulations suggests that the simultaneous presence of thermal effects and of interlayer defects, lowering significantly the activation energy barrier, causes a considerable reduction of the static friction threshold. An unexpected dependence on load is also predicted and related to the characteristic anticorrugation features of the Xe/Cu interaction. The mechanisms of dissipation during sliding are investigated by measuring the slip time.

[1] T. Coffey and J. Krim, *Phys. Rev. Lett.* 95, 076101 (2005).

Understanding the cleavage of diamond from the bond breaking

Pablo Pou[1,2], Rubén Pérez[2] y and Peter Gumbsch[1]

[1]*Kalrsruhe Universitaet, Germany*

[2]*Universidad Autonoma de Madrid, Spain*

First principles simulations provide the basis for the critical assessment of the different mechanisms proposed so far to explain the highly selective preference of diamond to fracture in the {111} set of planes. Our crack tip stability calculations for different crack orientations in the (111) and (110) planes show that cleavage in diamond is controlled by energy barriers to bond breaking that lead to lattice trapping of the crack. This conclusion is also supported by the differences found between the (111)and the other low-index diamond planes in the cohesive force function, calculated as the distance derivative of the energy per unit area required to separate two rigid slabs along their surface normals. This approach, that focuses on the accurate determination of the bond force non-linearity, provides an alternative to full fracture simulations in order to characterize the lattice trapping, and thus, the fracture behavior of materials.

Towards the synthesis of fullerenes: triazafullerene adsorption on noble metal close packed surfaces

G. Biddau[1], M. Basanta[1], J. Ortega[1], R. Pérez[1], G. Otero[2], B. Gómez-Lor[2], J.A. Martín Gago[2]

[1]*Universidad Autonoma de Madrid, Spain*

[2]*Instituto de Ciencia de Materiales de Madrid, CSIC, Spain*

Combining STM, XPS and NEXAFS measurements with first principles calculations, we study the adsorption of C57H33N3 on Au(111) and Pt(111) surfaces, and the possibility of closed fullerene formation by thermal annealing using these molecules as precursors. For room temperature deposition and molecular coverages from 0.1 ML to 5 ML, we found that the molecules diffuse on the Au(111) surface and thermal annealing (uo to 800 K) leads to occasional formation of triazafullerenes C57H2N3. When Pt(111) is used as substrate, the molecule is well anchored to the surface at room temperature, rending possible the observation of molecular orbitals, and the formation efficiency is close to 90% at 675 K. Large scale first principles local orbital DFT calculations, provide insight into these experimental results. Differences in mobility on Au(111) and Pt(111) are explained by the adsorption energetics, and traced back to the different surface reactivity. Molecular dynamics simulations, based on temperature-induced deshydrogenation, suggest a possible pathway for the formation of closed fullerenes.

First-principles study of the cubic-SiC(100) - 4x2 surface

D. González , P. Jelínek , J. Ortega

Universidad Autonoma de Madrid, Spain

We investigate the atomic scale structure and electronic properties of the Si-terminated SiC(001)-c(4x2) surface of cubic silicon carbide. This surface is known to undergo a reversible c(4x2) ↔ (2x1) phase transition at a temperature near 400 o C. The atomic structure of the low temparature phase, i.e. the β-SiC(001)-c(4x2) surface, is still under strong debate. Two are the main models under discussion: in the first model, proposed on the basis of experimental STM images, Si atoms form Si-Si dimer rows having alternatively up and down dimers (AUDD) [1]. The second model, the missing row asymmetric dimer (MRAD) model, was suggested on the basis of first-principles total energy calculations [2]. We have analyzed using an efficient first-principles molecular dynamics technique [3] these atomic models, as well as possible variants, obtaining two other atomic structures that are competitive with the AUDD and MRAD models. In order to discriminate between these four atomic models we have also calculated their corresponding theoretical STM images, that are compared in detail with the experimental evidence [1].

[1] P. Soukiassian et al., Phys. Rev. Lett. 78, 907 (1997); P. Soukiassian, Materials Science and Enginnering B 96, 115 (2002).

[2] W. Lu, P. Krüger and J. Pollmann, Phys. Rev. Lett. 81, 2292 (1998); J. Pollmann and P. Krüger, J.Phys.:Condens. Matter 16, S1659 (2004).

[3] J.P. Lewis et al., Phys. Rev. B 64, 195103 (2001); P. Jelínek et al., Phys. Rev. B 71, 235101 (2005).

Density functional embedding for molecular systems

Marcella Iannuzzi

Paul Scherrer Institute, Switzerland

We introduce a density functional based embedding method for the study of molecular systems in condensed phase. The system is partitioned in molecular subunits, which are individually treated by standard Kohn–Sham method by calculating the electronic density on small molecular grids. The necessary correction to include intermolecular interactions is introduced by an embedding potential derived from orbital-free density functional theory, by using kinetic energy functionals. The method leads to a linear scaling electronic structure approach that maps naturally onto massively parallel computers. Molecular dynamics simulations of water at room conditions result in a liquid with unstructured second solvation shell. The application to more weakly interacting molecular systems, like liquid acetronile, shows extremely satisfactory agreement between the full KS approach and the embedding approach. Improvements of the methodology should consider the neglected orthogonality condition betweem molecular orbitals belonging to differen molecular units. Extentions of the method will address the calculation of properties (spectroscopy) and the application to solid state.

[1] M. Iannuzzi, B. Kirchner, J. Hutter, Density Functional Embedding for Molecular Systems, Chem. Phys. Lett., vol. 421. 16-20, 2006.

[2] P. Cortona, Phys. Rev. B,, vol. 44, 8454 (1991).

[3] J. Wesolowski, J.Chem.Phys., vol. 106, 8516 (1997).

Enhanced chemical reactivity of gold nanowires

Pavel Jelinek, Rubén Pérez, Jose Ortega and Fernando Flores

Institute of Physics CAS, Czech Republic

Formation, exceptional stability and structure of pure one-dimensional gold atomic chains has been received a lot of attention last years. Experimental measurements show as significant changes of the conductance properties of atomic chains in presence of H_2 atmosphere [1] and recently work [2] reports experimental evidence for atomic chain formation strongly enhanced due to oxygen incorporation. For detail insight, we have carried out extensive first principles simulations, using fast local orbital DFT code FIREBALL, of the whole stretching process of Au nanocontacts combined with a Keldysh-Green's function approach for the electronic transport [3]. Our first principles simulations of the deformation path of a clean gold atomic contact show gradual formation of a mono-atomic chain with up to 4 atoms. As second step, we have studied possible adsorption and dissociation processes of H_2 molecule. In addition, we have performed simulations of the deformation process of Au nanocontact with oxygen molecule/atom to find possible tendency to be incorporated into the chain during the elongation process. In the case of H_2 molecule, our results [4] show how the molecule tends to dissociate on the Au chains and reduces significantly the conductance to values around ~0.6 G0 in very good agreement to experimental values [2]. In the case of O_2 , we observe an incorporation of the molecule into the mono-atomic chain along the stretching process forming longer chains according to the experimental observations [2]. Both cases point out strong chemical reactivity of gold atomic chain, in contradiction to well known nobility of gold material [5].

[1] Sz. Csonka et al, Phys. Rev. Lett. 90, 116803 (2003).

[2] W. H. A. Thijssen et al, Phys. Rev. Lett. 96, 026806 (2006).

[3] P. Jelinek et al, Nanotechnology 16, 1023 (2005).

[4] P. Jelinek et al, Phys. Rev. Lett. 96, 046803 (2006).

[5] B. Hammer, J.K. Norskov Nature 376, 238 (1995).

Interstitials in FeCr studied by Density Functional Theory

Peter Klaver, P. Olsson, M. W. Finnis

Queen's University Belfast, United Kingdom

Density Functional Theory calculations have been used to study relaxed interstitial configurations in FeCr alloys. The ionic and electronic ground state of 63 interstitial structures has been determined. Interstitials were placed in FeCr alloys with 9 to 14 atom percent Cr in which the Cr atoms were either monatomically dispersed or clustered together. The distance between the interstitials and Cr atoms was varied within the 4x4x4 bcc unit cell supercells. It is shown that Cr atoms at some distance from the interstitial can still influence the interstitial formation energy considerably. The multi-body nature of the Cr-Cr interactions in FeCr causes the Cr-interstitial interaction to be strongly concentration-dependent. Cr-interstitial binding energies calculated at dilute Cr concentrations can change by up to 0.5 eV and even change sign when recalculated at higher Cr concentrations. Determining the exact nature of the Cr-interstitial interaction is further complicated by the fact that FeCr alloying effects contribute more to the total formation energy than Cr-interstitial interactions. The long-range influence is not due to the interstitial strain field protruding into Cr-rich parts of the supercells. Instead, it is possible that some aspect of the electronic structure is responsible for changing the formation energies, although the Fermi-level and band energies were found not be the sole governing parameter. Our observations are likely to prove a serious challenge in the construction of FeCr force field potentials. Some patterns should not be too difficult for any potential to reproduce, e. g. the energy differences between different dumbbell orientations are quite independent from the configuration of Cr atoms that are slightly further away from the interstitial. Also, Cr atoms that are slightly further away from the interstitials seem to have little influcence on any aspect of the interstitial, as long as they are clustered together. However, monatomically dispersed Cr atoms do have a strong, long-range influence on the interstitials, so any empirical potential should not only be concentration-dependent, but should also be aware of the clustered/dispersed nature of the Cr. This observation, combined with the long-range, multibody, concentration-dependent nature of the Cr interactions will likely prove difficult to reproduce with a computationally cheap empirical potential.

Hydrogen damage in metals: Constrained molecular dynamics and Monte Carlo simulations of Superabundant vacancies

Döme Tanguy, E. Vamvakopoulos

CNRS, UMR 5146, Ecole des Mines de Saint-Etienne, France

Study of In adsorption on a In-rich a2(2x4) InGaAs surface on GaAs(001)

Marcello Rosini and Rita Magri

CNR-INFM-S3 and Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A, I-4100 Modena, Italy

The study of adatom diffusion and island nucleation on surfaces is a fundamental step to understand thin layer formation and morphology. In particular, it can shed light on the formation mechanisms of self-assembled nanostructures on surfaces. Here, we address one of the most studied systems: InAs quantum dots grown on a GaAs(100) substrate [2,3], where the lattice mismatch between InAs and GaAs is of the order of 7%. The calculation of the surface diffusion coefficient is a problem often tackled using multi-scale modeling approaches. The energy barriers between the adatom adsorption sites are calculated within a first-principles approach using a wide set of DFT calculations, while the diffusion simulation over larger time and space scales is then performed using a kinetic Monte Carlo Method. The first step is to calculate the surface equilibrium structure and the adatom adsorption sites as a function of the composition and related stress of the surface. We have considered a InAs layer, of thickness 1.75 monolayer (ML), grown on a GaAs(001) buffer. The surface is a2(2x4) reconstructed, that is supposed to be the stable reconstruction for a compressively strained InAs, such is the considered layer when the InAs deposition exceeds 1 ML [4]. The first-principles pseudopotential calculations were performed using the ESPRESSO simulation package. We have investigated the potential energy surface (PES) experienced by the In adatom, finding three adsorption sites and have calculated the potential barriers between them. The most stable adsorption site is found when the In adatom can bond to the As in-dimer on one side and to one surface In atom on the other side, thus saturating three bonds and completing the cation last layer. These results will be then used to simulate In surface diffusion.

[1] I. N. Stranski and L.Kastranow, Sitzungsber. Akad. Wiss. Wien, Math Naturwiss. Kl. IIb 146, 797 (1938).

[2] B. A. Joyce, D. D. Vvedensky, G. R. Bell, J. G.Belk, M. Itoh, and T. S. Jones, Mater. Sci. Eng B67, 7 (1999).

[3] J. G. Belk, C. F. McConville, J. L. Sudijono, T. S. Jones, and B. A. Joyce, Surf. Sci. 387, 213 (1997).

[4] F. Patella, A. Sgarlata, F. Arciprete, S. Nufris, P. D. Szkutnik, E. Placidi, M. Fanfoni, N. Motta, and A. Balzarotti, J.Phys-Condens Mat. 16 S1503 (2004).

Effects of impurities on cohesion at $\Sigma 5(210)$ grain boundary of magnetic metals

Elwira Wachowicz, T.Ossowski and A. Kiejna

Institute of Experimental Physics, University of Wroclaw, Poland

Impurities at grain boundaries can lead to embrittlement or to strengthening of the material. We have studied the B, N and O impurities placed in interstitial and substitutional positions at symmetric $\Sigma 5(210)$ Fe grain boundary (GB). The full relaxation of supercell shape and volume results in a stable asymmetric grain boundary. We found that nitrogen in both interstitial and substitutional position is a cohesion enhancers while oxygen and boron are embrittlers. In all cases we observe big shifts ($0.47\div 2.33$ \AA) of grains with respect to each other. The equilibrium distance between the grains is decreased for impurities in substitutional positions and increased for atoms in interstitial places with respect to the relaxed clean GB. The magnetic moments of Fe atoms at grain boundary are increased and they tend to the bulk value in the middle of the grain in an oscillatory way. We also present preliminary results on grain boundary cohesion in antiferromagnet chromium.

From individual defects to microstructures

Fabrizio Cleri

Institute of Microelectronics, Electronics & Nanotechnology, University of Lille I, France

I will discuss the assemblage of a multiscale strategy for the study of microstructure evolution in polycrystalline materials. Starting from atomistic models of isolated defects (dislocations, grain boundaries, microcracks, etc.), a hierarchy is constructed to obtain the time and length scale parameters for collective degrees of freedoms. The latter describe the defects and their interaction, in a class of mesoscale models based on a variational formulation of the dissipated power.

[1] F. Cleri, Physica A, 282 (2000) 339

[2] F. Cleri & G. D'Agostino, J. Mat. Res. 17 (2002) 17

[3] F. Cleri, Phys. Rev. B65 (2002) 014107

[4] A. Satta et al., J. Phys. Cond. Matt. 14 (2002) 13003

[5] F. Cleri, Comp. Phys. Comm. 169 (2005) 44

[6] V. Sansalone et al., Acta Mat. 54 (2006) 3485

Computational tools for modeling and simulation of nanoscale systems

Reinier Akkermans

Accelrys Ltd, United Kingdom

We present various computational tools that can aid research of nanoscale systems, by providing concrete examples of multiscale modeling workflows, in which mesoscale models are contructed from atomistic data, and mesoscale simulation methods are used to generate input for finite-element calculations. The link between the micro- and mesoscale is discussed into more detail, in particular the coarse-graining route via the Flory-Huggins theory of mixtures. We investigate a simple method to estimate the Flory-Huggins interaction parameters from force field calculations, based on sampling the density-of-states of molecular clusters in the space spanned by coarse-grained coordinates. We show how we use the density-of-states to calculate the excess free energy of mixing, and how this leads to mesoscale interaction parameters.

[1] R.L.C. Akkermans & P.B. Warren, Multiscale modelling of human hair, Phil. Trans. A 362, 1783-1793 (2004)

[2] R.L.C. Akkermans, The Langevin equation for generalized coordinates, Lect. Notes Phys. 49, Eds. B. Leimkuhler et al., 155-165 (2006)

[3] R.L.C. Akkermans & W.J. Briels, Coarse-grained dynamics of one chain in a polymer melt, J. Chem. Phys. 103, 6409-6422 (2000)

[4] A. Maiti, J.T. Wescott & P. Kung, Nanotube-polymer composites: insights from Flory-Huggins theory and mesoscale simulations, Mol. Sim. 31, 143 (2005)

[5] A. Maiti, J.T. Wescott & G. Goldbeck-Wood, Mesoscale modelling: recent developments and applications to nanocomposites, drug delivery and precipitation membranes, Int. J. Nanotechnology 2, 198 (2005)

[6] S. McGrother, G. Goldbeck-Wood & Y.M. Lam, Integration and modelling at various length and time scales, Lect. Notes Phys. 642, 223-233 (2004)

Metal adhesion at oxide ceramic interfaces

J.I. Beltrán, S. Gallego and M.C. Muñoz

Instituto de Ciencia de Materiales de Madrid,CSIC, Spain

Heterogenous metal-ceramic systems are employed in multifunctional devices, which exploit the properties of composite materials formed by dissimilar constituents. In these materials the interface strength is crucial in determining the macroscopic properties and therefore they are significantly dependent on interface adhesion. We have performed an ab-initio systematic investigation of the interface properties and adhesion between transition metals and oxide ceramics, which allows us to extract qualitative trends on the dependence of the adhesion on the structure, stability and metal electronic charge

[1] M.C. Muñoz, S. Gallego, J.I. Beltrán and J. Cerdá, Surface Science Reports 61,303 (2006)

Relaxation of semiconductor interfaces by molecular dynamics using enhanced bond order potentials

Kurt Scheerschmidt and Volker Kuhlmann

Max Planck Institute of Microstructure Physics, Weinberg2, 06120 Halle, Germany

Accurate empirical potentials are needed to study atomic processes via molecular dynamics (MD) simulations at time and length scales relevant for nanoscopic processes such as surface interaction during wafer bonding or relaxation of quantum dots.

Starting from the tight binding model (TB) an analytical expression for the bond order potential (BOP) is derived, which is related to the electronic density. In the crystal the attraction due to formation of electronic bonds is balanced by the repulsion (overlap & coulomb) as well as the energetic penalty incurred by electronic promotion. The analytic derivative of this cohesive energy describes the forces acting on each atom, which are then used to integrate the Newtonian equations of motion to study the MD. Expression for the σ bond order has been improved by including intermediate π bonds and on-site cross terms. Along with the coordination-dependent expression proposed for the promotion energy, the BOP4^+ with 4^{th} moments of the density accurately describes covalent bonds while scaling linear with the system size.

MD simulations applying BOP4^+ to study the generation of wafer bonded interfaces, which is like a crack closure process influenced by the surface step structure, roughness, defects, adsorbates, and the misalignment of the wafers, demonstrate the validity and advantage of the new potential.

[1] A. Horsfield, P. Godwin, D. Pettifor and A. Sutton, Phys. Rev. B 54:15773 (1996)

[2] D. Pettifor, M. Finnis, D. Nguyen-Manh, D. Murdick, X. Zhou and H.Wadley, Mater. Sci. Eng. A:365, 2 (2004)

[3] V. Kuhlmann and K. Scheerschmidt, submitted to Phys. Rev. B (2006)

Multiscale Hybrid Simulations of Brittle Fracture

James Kermode, Gabor Csanyi, A. De. Vita, M.C. Payne

Cavendish Laboratory, United Kingdom

The Learn on the Fly (LOTF) molecular dynamics scheme, which combines quantum-mechanical embedding and classical force model optimisation is applied to the brittle fracture of silicon. Dynamical simulations of cracks moving in the (111) cleavage plane show a novel sub-critical crack tip reconstruction, similar to the Pandey 7-5 surface, that delays the onset of fracture by increasing the lattice trapping barrier.

This poses the question: what is the equilibrium shape of the crack-tip? There is a competition between the local chemical energy required to break bonds and the elastic energy recovered by the formation of such a reconstruction. Since the latter is distributed over thousands of atoms, hybrid simulation is the ideal tool to investigate such truly multiscale problems.

The LOTF method is also currently being applied to the fracture of diamond and of graphene sheets.

A cohesive zone model for stress corrosion cracking in ceramic polycrystals

Rafael Estevez, M. Romero de la Osa, C. Olagnon, J. Chevalier, C. Tallaron, L. Vignoud

INSA Lyon / GEMPPM, France

Fracture in oxyde based ceramics is time dependent and three regime can be distinguished: beyond a load threshold; (I) the crack velocity increases with the charge, (II) stabilizes and (III) unstable crack propagation takes place thus defining the material toughness. In the present study, we focus on the description of the regime I. While the bulk response is linear elastic at room temperature, the mechanism underlying rupture combines a chemical and a mechanical action at the crack tip. The time and temperature dependency originates from a reaction-rupture process which is both thermally activated and stress dependent. In the case of ceramics, the water is involved in the chemical effect for bond breaking through a molecular process proposed by Michalske (1983, JACS). We present a cohesive zone description for the time dependent reaction-rupture process. We then show some results related to the time dependent intergranular failure in a 2D polycrystal.

Participant List

Fabrizio Cleri (fabrizio.cleri@isen.fr)
Institute of Microelectronics, Electronics & Nanotechnology, University of Lille I France
Gabor Csanyi (gabor@csanyi.net)
University of Cambridge United Kingdom
Alessandro De Vita (devita@units.it)
King's College London, UK and CENMAT UTS United Kingdom
Oscar Custance (oscar@afm.eei.eng.osaka-u.ac.jp)
Graduate School of Engineering, Osaka University Japan
Peter Gumbsch (gumbsch@iwm.fraunhofer.de)
Fraunhofer Institute for Mechanics of Materials IWM Germany
Alexis Baratoff (alexis.baratoff@unibas.ch)
Uni Basel, Institute of Physics Switzerland
Noam Bernstein (noam.bernstein@nrl.navy.mil)
Naval Research Laboratory United States
Joost Frenken (frenken@physics.leidenuniv.nl)
Leiden University Netherlands
Nicolas Agrait (nicolas.agrait@uam.es)
Universidad Autonoma de Madrid Spain
Giovanni Ciccotti (giovanni.ciccotti@roma1.infn.it)
Dipartimento di Fisica, Universita' Italy
Jörg Behler (jbehler@phys.chem.ethz.ch)
ETH Zurich Switzerland
Stefaan Cottenier (stefaan.cottenier@fys.kuleuven.be)
Katholieke Universiteit Leuven Belgium
Giulio Biddau (giulio.biddau@uam.es)
Universidad Autonoma de Madrid Spain
Mauro Ferrario (ferrario.mauro@unimo.it)
Dipartimento di Fisica, Università di Modena e Reggio Emilia Italy
Albert Bartok-Partay (ab686@cam.ac.uk)
University of Cambridge, Cavendish Laboratory, TCM Group United Kingdom
Daniel Gonzalez (daniel.gonzalez@uam.es)

Universidad Autonoma de Madrid Spain
Rafael Estevez (Rafael.Estevez@insa-lyon.fr)
INSA Lyon / GEMPPM France
Reinier Akkermans (ReinierA@Accelrys.com)
Accelrys Ltd United Kingdom
Maria Samaras (maria.samaras@psi.ch)
Paul Scherrer Institiute Switzerland
Mike Payne (mcp1@cam.ac.uk)
University of Cambridge United Kingdom
Jingzhe Pan (jp165@le.ac.uk)
University of Leicester United Kingdom
Ugo Valbusa (Valbusa@fisica.unige.it)
Physics Department, University of Genova Italy
Ruben Perez (ruben.perez@uam.es)
Universidad Autonoma de Madrid Spain
Karsten Reuter (reuter@fhi-berlin.mpg.de)
Fritz-Haber-Institut der Max-Planck-Gesellschaft Germany
Erik van der Giessen (E.van.der.Giessen@rug.nl)
University of Groningen Netherlands
Sidney Yip (syip@MIT.EDU)
Massachusetts Institute of Technology United States
Andrew Minor (AMinor@lbl.gov)
Lawrence Berkeley National Laboratory United States
Jacqueline Krim (jkrim@unity.ncsu.edu)
North Carolina State University United States
Bo Persson (B.Persson@fz-juelich.de)
Forschungszentrum Juelich GmbH, Institut fuer Festkoerperforschung Germany
Eric Vanden Eijnden (eve2@courant.nyu.edu)
Courant Institute of Mathematical Sciences United States
Berend Smit (b.smit@cecam.fr)
CECAM, Lyon France
Carla Molteni (carla.molteni@kcl.ac.uk)
Kings College London United Kingdom
Jörg Meyer (meyer@fhi-berlin.mpg.de)
FHI Germany
Elwira Wachowicz (elwira@ifd.uni.wroc.pl)
Institute of Experimental Physics, University of Wroclaw Poland
Alex Shluger (a.shluger@ucl.ac.uk)
University College, London United Kingdom
Lev Kantorovich (lev.kantorovitch@kcl.ac.uk)
Physics, King's College London United Kingdom
Michael Urbakh (urbakh@post.tau.ac.il)
School of Chemistry, Tel Aviv University Israel

Matthias Krack (krack@phys.chem.ethz.ch)
ETH Zurich Switzerland
Thomas Kühne (tkuehne@phys.chem.ethz.ch)
ETH Zü rich Switzerland
Pablo Pou (pablo.pou@uam.es)
Universidad Autonoma de Madrid Spain
Gilles Perrin (gilles.perrin@ifp.fr)
IFP France
Kurt Scheerschmidt (schee@mpi-halle.de)
Max-Planck-Institut fü r Mikrostrukturphysik Germany
Johann von Pezold (pezold@mpie.de)
Max Planck Institute of Iron Research Germany
Rita Magri (magri@unimore.it)
Dept. of Physics - Univ. Modena Italy
Izabela Szlufarska (izabela@engr.wisc.edu)
University of Wisconsin - Madison United States
Marcella Iannuzzi (marcella.iannuzzi-mauri@psi.ch)
Paul Scherrer Institute Switzerland
Maria Clelia Righi (mcrighi@unimore.it)
Dipartimento di Fisica, Universita' di Modena e Reggio E. Italy
James Kermode (jrk33@cam.ac.uk)
Cavendish Laboratory United Kingdom
Tomasz Ossowski (osa@ifd.uni.wroc.pl)
Institute of Experimental Physics Univesity of Wroclaw Poland
Carmen Muñoz (mcarmen@icmm.csic.es)
Instituto de Ciencia de Materiales de Madrid,CSIC Spain
Peter Klaver (t.p.c.klaver@qub.ac.uk)
Queen's University Belfast United Kingdom
Laurent Pizzagalli (Laurent.Pizzagalli@univ-poitiers.fr)
CNRS France
Pavel Jelinek (jelinekp@fzu.cz)
Institute of Physics CAS Czech Republic
Nele Moelans (nele.moelans@mtm.kuleuven.be)
Katholieke Universiteit Leuven Belgium
Emmanuel Vamvakopoulos (evamvak@yahoo.com)
CECAM-ENS LYON France
Döme Tanguy (tanguy@emse.fr)
CNRS, UMR 5146, Ecole des Mines de Saint-Etienne France