

## **PROPOSAL FOR A CECAM/Psi-k WORKSHOP**

### **COVER SHEET**

Title of this meeting: “ Multiscale approaches to Nanomechanics”

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Tentative Dates: Early Winter 2007 (Arrival day: )  
(Departure day: )

Tentative Venue: CECAM (Lyon, France)

Duration and Size: 3 days for 60 participants

## PROPOSAL SUMMARY

### Scientific Content

This meeting is focused on the application of first-principles computer simulations to the study of the microscopic aspects that determine the mechanical behaviour of materials. This includes the structure and interaction of the atomic-scale defects (crack tips, dislocation cores, grain boundaries, etc) involved in macroscopic failure, the mechanical and electronic transport properties of nanocontacts and biological molecules, and the interaction between nanoasperities (tips) and surfaces which is behind both the operation of the scanning probes and the tribological contact between two materials. All these problems share an essentially multi-scale nature: the breaking and formation of atomic bonds are **dynamically** coupled by long-range interactions (elasticity) to the macroscopic boundary conditions (deformation, load) imposed. Thus, a reliable prediction of mechanical properties requires the coupling of first-principles simulations, describing the atomic bonding with chemical accuracy, with classical atomistic and continuum descriptions. The mechanical and transport properties of nanometer-size contacts and biomolecules, experimentally characterized in detail in the last few years, provide a natural testing ground for the development of theoretical methodologies designed to bridge the length and time scales.

The meeting will face the current challenges in Nanomechanics: merging quantum mechanical methods with the complementary but largely separate methodologies dealing with the different larger scales; bridging the gap between simulations and experiments; and providing a necessary unified perspective that spans beyond the boundaries of traditional scientific disciplines.

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## PROPOSAL DESCRIPTION

### Scientific Content

The mechanical properties of materials are ultimately determined by events occurring at the atomic scale. While this is acknowledged in the introduction of most Material Science textbooks and monographs on mechanical properties of materials, little attention is still paid to these microscopic aspects in the following sections, which focus on a macroscopic description based on continuum mechanics.

Atomistic simulations (with interatomic interactions described by empirical potentials) have recently gained an increasingly important role in the understanding of mechanical properties. They represent a giant step forward, providing essential tools for capturing some qualitative features of mechanical behaviour (e.g. lattice trapping, i.e. the existence of a range of loads where the crack is stable), which are lost in a purely continuum description.

However, classical interatomic potentials are unable to capture some of the most basic features of the formation and breaking of atomic bonds, which can only be properly described using quantum mechanics. For example, even the most sophisticated interatomic potential, fitted to reproduce the mechanical properties of Si bulk phases, fails to reproduce the brittle character of its fracture. Both the developments of efficient algorithms and the increase in computer power have made possible to extend quantum mechanical simulations (based mostly on density functional theory) from figurative calculations on a handful of atoms to several-hundred-atom systems, with nearly chemical accuracy, hence approaching system sizes relevant for material science problems. The last ten years have seen the application of first-principles simulations, with a careful choice of models and boundary conditions, to “classical” mechanical problems, such as crack propagation and grain boundary sliding.

The trend in Condensed Matter Physics towards probing matter on shorter and shorter scales has naturally focused our attention to the microscopic aspects relevant at the nanometer scale. Scanning probes have led this revolution, by extending classical characterization techniques (such as indentation testing) to the nanometer scale, providing completely new information channels (such as the local conductance, i.e. the source contrast in the STM), and giving access to new physical phenomena (such as the conductance quantization in atomic or molecular nanocontacts). This revolution has reached other “classical” fields like wear (polishing, cutting) and tribology. The atomic force microscope (AFM) and the quartz-crystal microbalance have opened the field of nanotribology, which provides atomistic information on the mechanical processes and atomic-scale dissipation mechanisms taking place in the many nanoasperities present in the contact between two surfaces.

Scanning probes allow us to manipulate matter at the atomic scale. STM has been used to move atoms and molecules over surfaces, while the mechanical properties of some important biological molecules (e.g. DNA) and structures (e.g. the molecular motors packing DNA on some viruses) have been measured with AFMs and optical tweezers.

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 first-principles simulations, addressing the mechanical and transport properties of systems of increasing size and complexity, are currently meeting. While microscopic considerations are crucial, these problems are characterized by the relevance of many different length scales. Quantum mechanics is essential for the shorter length scales (the formation and breaking of bonds), but one cannot forget the long range interactions: elasticity if you are dealing with the propagation of a crack and the mechanical properties a nanocontact, electrostatics if you want to describe the influence of the charged ligands surrounding the active site of a biomolecule (e.g. the Fe ion in hemoglobine) in its response and function.

The theoretical challenge comes from the fact that these problems are not amenable to a hierarchical or sequential treatment of the different length (or time) scales: we cannot restrict ourselves to do simulations on one scale (e.g. first-principles calculations of diffusion barriers) and feed the results to the next step up the length/time scale ladder (e.g. kinetic Montecarlo simulations of growth). In our case, a concurrent approach is needed, since we are dealing with problems where the different scales interact dynamically: due to the load transmitted by the elastic field, a brittle crack advances by the breaking of the atomic bond at its tip, but this bond breaking triggers a long-range reordering of the surrounding atoms as the elastic displacements have to be consistent with the new position of the crack elastic field singularity.

The study of mechanical properties of materials (cracks, dislocations, grain boundaries etc.) has been the natural playground for the theoretical development of multiscale methods, which try to couple an atomistic description (based on classical force fields) with a continuum description of the elastic response (based on finite-element methods). The hand-shaking between these two descriptions is still a matter of active research. The next and major challenge is the inclusion of an inner level, where the description is fully quantum mechanical in order to account properly of bond formation. The connection between the QM and the atomistic descriptions leads to the issues of saturation and embedding of the system used for the QM calculation, that have been explored in recent years by computational chemists (e.g. Model potentials and hybrid QM/MM methods) and physicists (Green's function approaches).

Research on mechanical properties is truly interdisciplinary, and recognising and responding to this is the key to progress. There are several facets to explore: no single simulation approach or methodology will provide all the answers, and problems need skills and knowledge from across traditional disciplines. Moreover, it is increasingly clear that experiment and theory must concert their efforts. Accordingly, this meeting will gather eminent researchers from physics, chemistry, materials, and life sciences. The conference will provide a common playground for all these different communities. From the theoretical point of view, ab initio practitioners will benefit from an overview of the work done on the atomistic-continuum coupling and the more interesting problems in materials science (microscale), while the material scientists will get the flavour of the systems and problems that can now be tackled with current first-principles and multiscale QM-atomistic-continuum methods. Experimental contributions will illustrate the relevant problems on the nanometer scale, and the interaction with the theorist will help

to define model experiment/simulations where theory (equipped with these new multiscale tools) and experiment can be compared. This rich, stimulating and synergetic environment is the best to realize the ultimate goal of the meeting which is to advance the simulation approach, but also to produce real and exciting progress in the broader area of Materials Properties, with important technological and industrial implications.

Nanotechnology still lacks the set of well-established concepts that characterize a mature discipline. This meeting has the potential to contribute significantly in defining the core issues and challenges that should pervade the future development of Nanomechanics. Specifically, we hope to encourage new cross-disciplinary projects, identify key methodological areas in need of development, achieve a better appreciation of the nature of these scientific problems by understanding the viewpoints of other disciplines, strengthen and extend international networks of support and collaboration.

There are major opportunities in Europe for progress in this research field. Europe is at the forefront of the development and application of computer simulation techniques, and many research groups and individuals are of leading international standing. Our collaborative “network” approach is a great strength, which is envied elsewhere: it will be essential in meeting the challenges identified in this proposal. Methods are becoming mature and well established, and progress is evident on many fronts which will lead to advances in efficiency, accuracy and range of applicability. Furthermore, experimentalists are realising what insight and value is added to their research when simulation is a part of it. The need now is to think and act on a bigger scale, one which embraces the skills of all relevant disciplines, and one which can tackle the difficult and complex science that lies ahead.

## **Format & Programme Content**

The programme is mostly based on 50 minutes (including 15 minutes discussion) assisted keynote presentations delivered by the speakers listed below, where they will provide a

general overview of the topic, identify strengths and weaknesses of their particular research method(s), and give opinions on promising developments.

The keynote speakers and session chairs (see draft programme below) have been chosen among the leading experts in the different fields, covering a broad range of disciplines. Some of them (like Prof. P. Gumbsch, also Director of the Fraunhofer Institute for Mechanical Properties in Fribourg; Prof. E. A. Carter, and Prof. Sidney Yip) have a strong involvement in applied research and will brought the technological and industrial perspective into the meeting. The significant contribution from the experimental side reflects the interdisciplinary character of the meeting and the relevance given to the interplay between theory and experiment.

The current proposal is based on an extended proposal for a full 5-days Conference, that was well evaluated and accepted for funding by ESF, but did not finally take place due to the financial problems of the whole ESF conference programme in 2003. The scope of the conference has been focused and the programme condensed in only three days in order to cope with possible budget constraints and, more importantly, to facilitate that all the delegates will attend the whole conference. This is a key consideration in making sure that the presentations and discussions (there will be ample opportunity for extended and informal discussion during scheduled breaks) will allow substantial scientific interactions to be built up.

To ensure full and active participation, young researchers will be encouraged to present their work in poster sessions. This will provide a natural means of introducing themselves to scientists active in their field.

### **Budget**

— Standard budget for a 3-day activity provided by CECAM.

In addition, we expect contribution from the European networks or programmes directly related to simulation in order to meet the costs involved in a larger event like this.

- Psi-k European Network, funded through the ESF programme on “Towards Atomistic Materials Design.
- The recently approved SimBioMa programme, funded by the ESF.

### **Draft Programme** (Chairpersons in parenthesis)

This draft programme is intended to indicate the major areas of interest and possible speakers. The details should be considered as preliminary.

### **Atomic-scale defects: the challenge of coupling length scales**

(Peter Gumbsch, University of Karlsruhe, Germany; M. W. Finnis, University of Belfast, UK)

- Erik van der Giessen (University of Groningen, The Netherlands)  
*Micromechanics*
- Efthimios Kaxiras (Harvard University, Cambridge, USA)  
*First-principles applications to mechanical properties: stacking faults and dislocation mobility.*
- Karsten W. Jacobsen (Danish Technical University, Lingby, Denmark)  
*Atomistic simulations based on embedded potentials and the quasicontinuum method*
- Sidney Yip (MIT, Cambridge, USA)  
*Microscopic description of the onset of Plasticity*
- Alessandro de Vita (University of Trieste, Italy and EPFL, Laussane, Switzerland)  
*The learning-on-the-fly embedding (LOTF) method: Applications to brittle fracture*

### **Advances in Molecular Dynamics: Coupling time scales, simulation of energy transfer mechanisms and pressure/load conditions**

(G. Ciccotti, University of Rome, Italy ; B. Smit, CECAM, France)

- Daan Frenkel (FOM, Amsterdam, The Netherlands)  
*Simulating the complexity of biological systems*
- Gerbrand Ceder (MIT, Cambridge, USA)  
*Coarse-graining in both the length and time scales*
- Emily A. Carter (Princeton University, USA)  
*Ab initio Molecular Dynamics: understanding the degradation of metals via corrosion and embrittlement.*
- Michele Parrinello (Swiss Center for Scientific Computing, Manno, Switzerland)  
*Microscopic simulations of pressure/load conditions. Phase transformations.*
- Hannes Jonsson (University of Reykjavik, Iceland )  
*Long time scale simulations of complex systems*

### **Mechanical and Transport properties of nanomaterials, Nanocontacts, Nanotribology**

(U. Valbusa, University of Genoa, Italy; Uzi Landman, Georgia Tech, USA)

- Ernst Meyer (University of Basel, Switzerland)  
*Dynamic atomic force microscopy: Imaging, dissipation and manipulation*
- Jacqueline Krim (North Carolina State University, Raleigh, USA)  
*Friction at the atomic scale*
- B. Person (Forschungszentrum Julich, Germany)  
*Theoretical challenges in the study of friction.*
- Miquel Salmeron (LBNL, Berkeley, USA)  
*Structure, Dynamics and Manipulation of water on surfaces*
- Joost Frenken (Leiden University , The Netherlands)  
*Superlubricity*
- Nicolas Agrait (Universidad Autonoma de Madrid, Spain)  
*Mechanical and transport properties of nanocontacts*
- Elisa Molinari (INFM Center for nanostructures and biosystems at surfaces and University of Modena, Italy)  
*Theoretical modelling of DNA-based nanowires*
- A.P. Alivisatos (University of California, Berkeley, USA)  
*Nanocrystals*
- David Tomanek (Michigan State University, USA)  
*Nanomechanics and Nanoelectronics with carbon: A theoretical approach*

## **Research Training Measures**

### **Training Need**

First-principles simulation is no longer the domain of a few solid-state theorists. It has become one of the most powerful tools in fundamental studies of the chemistry and physics of matter at the atomic scale. It is increasingly applied in a diversity of fields, from earth science to catalysis to biochemistry. Thus, there is a large and growing demand for scientists trained in the theory and practice of first-principles methods.

First-principles applications to mechanical properties of materials require knowledge from many disciplines. Material science helps to identify the relevant problems and provides the background information (atomistic simulations and experimental results) needed to design meaningful first-principles simulations. Quantum Chemistry, Mechanical Engineering and Biochemistry share the expertise in embedding and multiscale methods design to couple different length scales. Researchers in this field need to meet those from relevant disciplines, to learn and to form collaborative relationships.

In the experimental community there is a growing understanding that first-principles calculations make indispensable contributions to not only our fundamental understanding of interfaces, but to the interpretation and guidance of experiments. It is increasingly clear that a combined approach is best, and this results in demand for simulation from experimentalists. This in turn leads to a training need, which is for young researchers who are not simulation experts or theorists may learn about first-principles theory and practice.

### **Training Impact**

This meeting will draw together internationally-eminent scientists from the many disciplines involved in the understanding and prediction of the mechanical properties of materials. It is designed to give access to their expertise and knowledge through extended, in-depth discussions. It is an unrivalled training experience for young researchers: few meetings span the necessary disciplines or allow the chance to spend several days with leading figures. In this field, industry is eager to take up first-principles methods and research. Reciprocally, academic research is often better-directed when researchers are aware of technological challenges. The industrial perspective will be brought by the keynote speakers and session chairs with a materials science profile.

The topic of this meeting is timely and there is enormous potential for progress over the next decade. This potential will be realised through collaborations and projects that cut across our current discipline boundaries. New developments in techniques and applications require the creative synergy of these collaborations. The impact of this meeting will stem from bringing together the experts and young researchers who will make this happen.