1. Title: Mineral Physics with Computation and Experiment

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2. Scientific content and why a workshop would be useful at this time.

Mineralogical problems involve a vast range of materials and behaviour, from simple minerals at extreme conditions (very high temperatures at very high pressures) to complex interactions between minerals, fluids, contaminants and bioorganisms. Hence, in Mineral Physics, there is not only a reliance on the fundamental methodologies of physics and chemistry, but also a significant overlap with materials science, engineering and the biosciences. Due to the need to answer challenging and relevant questions, the mineral sciences continue to act as a test-bed for many emerging theoretical and experimental techniques and motivate new advances.

Computer modelling of complex materials has progressed greatly over the last 10 years, and this has been well followed within the mineral sciences. Advances in computer technology have had a huge impact on our understanding of many processes, from free energies of minerals at the core-mantle boundary to mechanisms of mineral growth and dissolution at the Earth~s surface. Quantum mechanical techniques are now widespread but still have limitations in size and scope; empirical techniques are still used for many simulations. The effort currently focussed on ~eScience~ in many countries is now promising even greater resources for interdisciplinary studies of environmental systems. This will enable not only more powerful computer simulations but also stimulate the collaborative use of observational data from many sources. The wide range of existing computational approaches combined with new forms of collaboration presents a rich environment in which to develop new possibilities for uncovering the structures and mechanisms of complex mineralogical systems.

Experimental observations are also crucial to research in the geosciences and can occur on scales from the near-atomic to mesoscopic or even macroscopic scales, and on a range of systems from a single crystal to a sample with complex chemical or even biological components. Major advances in techniques such as NMR spectroscopy, synchrotron radiation, neutron scattering, phonon spectroscopy and laser-ablation based techniques are bringing significant benefits to the mineral sciences. However, understanding earth science processes ultimately demands insight on an atomic scale. Here computer simulations are essential to link experiments to conceptual models, whether by providing unequivocal interpretations or by doing separate ~computer experiments~ to avoid experimental constraints.

The complexity and diversity of mineralogical problems require the integration of theoretical, computational and experimental approaches. In previous meetings (beginning in 1997) the diverse needs and expectations of participants from the viewpoint of their different subfields have become evident during discussions of each presentation, and have helped to define the extent to which

- theory is sufficiently accurate to experiment to be useful
- experiment is sufficiently accurate to test theories

- both theory and experiment can address complex systems
- results from distinct computational approaches are comparable

The 2004 workshop, for example, resulted in an effort to use benchmark minerals to compare simulation codes and this initiative has now been funded by the UK National Institute for Environmental eScience. For this reason, invitees to the workshops, both past and planned, include code developers, those developing novel experimental techniques and users seeking to apply both approaches to mineralogical problems; in many cases participants may fall into more than one of these categories. The challenges presented during the workshop will therefore stimulate developments across the community.

The essential integration of experiment and theory is hindered by the fact, that many of the mineral sciences research groups in Europe are small and many new techniques are limited by facilities and/or expertise to one or two research groups. This was recognized on an European scale and has led to a ESF-EUROCORES, EuroMinScI. Two of the current proposers (SS and BW) were involved in this. The ESF EuroMinSci programme recognised that ~in order to capitalise on the recent advances in computer methods and new experimental methods it is vital to adopt an nterdisciplinary approach~ and to continue to bring new advances into the earth sciences. The planned workshop seeks to exploit the momentum of EuroMinSci to further collaboration and knowledge transfer. We wish to invite a speaker from each of the funded EuroMinSci projects, in order both to learn from the ways in which they are integrating theory and experiment and to ensure projects can take full advantage of emerging methodologies.

In all past workshops, presentations of computational and experimental research are made to scientists from both communities, in a single session. All speakers have been and will be required to make their talk accessible to those with a whole range of backgrounds, in order that other participants can then discuss ways in which their own research might benefit. As in the past, it is intended that presentations will be sufficiently detailed to germinate ideas for new collaborations and that there will be frequent opportunities for discussion to allow these ideas to be developed rapidly thereafter.

A continued interplay between experiment and theory will encourage debate between the communities as to the best ways to combine the two approaches, their relative accuracies and applicabilities and the advances that are most urgently required. For this reason the schedule will be arranged thematically, not according to the techniques employed. The scientific programme will mirror the EuroMinSci programme, ensuring that a wide range of approaches are considered. We therefore particularly consider the following topics:

(a) Behaviour at high pressures and temperatures, including phase transitions and thermoelastic properties, which still present challenges to both theory and experiment;
(b) Structures and properties of amorphous and disordered materials, which not only are hard to model at thermodynamic equilibrium but also involve non-equilibrium processes that are manifested differently in theory and experiment.
(c) Defects and microstructures, which substantially modify mechanical, electrical, and transport properties.
(d) Transport mechanisms (and thus kinetics) at the atomic length scale: e.g diffusion, defect migration, leaching, thermal and electrical conductivity, each of which have a role in the other processes listed.
(e) Trace elements and isotope partitioning, with implications for models of the Earth~s composition and evolution as well as environmental monitoring. Trace components also present problems to both theory and experiment and are thus worth of considerable discussion.

(f) Structure, properties and reactivities of mineral surfaces: interactions of thebiosphere, atmosphere and hydrosphere with the lithosphere all occur on mineral surfaces and understanding atomic-scale processes in these complex systems requires a wide range of experimental and computational approaches to be combined.
(g) Spectroscopy of minerals and the quantitative interpretation of spectra: relating spectroscopic data to the atomistic structure in a quantitative manner, taking into account spatial and/or temporal averaging, has only recently become possible due to advances in instrumentation and theory.

3. Tentative list of speakers

Experimentalists will be invited which represent the current active fields mentioned above. From the code developers, we wish to have at least one representative of each of the major codes currently used. We expect that from the majority of the EuroMinScI collaborative research groups at least one principal investigator will participate.

The current list of speakers we plan to invite is:
(* = 'confirmed')

* David Allan (Edinburgh) - high-pressure crystal growth (exp)
- Dario Alfe' (UCL) - Melting (theory)
* Emilio Artacho (Cambridge) - H2O/large structures/O(N)
- Patrick Cordier (Lille) - Rheology (exp)
* Stefano de Gironcoli (Trieste) - High-spin low-spin (theory) / Qm-ESPRESSO
* Przemek Dera (Geophysical Laboratory, Washington) - single crystal structures at MBar (exp)
* Lars Ehm (Stony Brook) - Laser heating (exp)
- Guillaume Fiquet (Paris) - High-spin low-spin transition (exp)
* Volker Heine (Cambridge) - always good to have
* Kersti Hermannson (Uppsala) - anharmonicity in hydrogen bonds (theo)
* Sandro Jahn (GFZ Berlin) - link between DFT and empirical potentials (theo)
* Karsten Knorr (Kiel) - high pressure powder diffraction (exp)
* Peter Kroll (Aachen) - predictions of reactions (theo)
- Georg Kresse (Vienna) - PAW
- Victor Milman (Accelrys) - CASTEP
* Chris Pickard (St. Andrews) - NMR (theo)
* Matt Probert (York) - quantum MD (theo)
* Keith Refson (CCLRC-RAL) - phonons (theo)
- Karlhein Schwarz (Vienna) - electron densities/bonding in minerals (theo)
* Sandro Scandolo (Trieste) - free energies (theo)
* Gerd Steinle-Neumann (BGI Bayreuth) - high pressure phases (theo)
* Michele Warren (Manchester) - environmental studies (theo)
* Bjoern Winkler (Frankfurt) - high pressure/high temperature neutron diffraction (exp)

+ 5 experimentalists from EuroMinScI
+ 3 modellers from EuroMinScI

4. The number of participants

In the past, about 25 - 30 researchers have attended the 'Psi-k/CECAM' Mineral Physics workshops. This was very effective, as this allowed for each participant to give a full presentation and have enough time for discussions. We would therefore like to continue to limit the participation to about 30 participants.

5. Plans for a tutorial element and for attracting new researchers into the subject of the workshop.

New participants to the field will be attracted to the workshop by our invitation policy. This has worked extremely well in the past. For the planned workshop, there is a large new pool of potential participants, namely those involved in the EuroMinSci-EUROCORES. The final funding decision will be taken in September, and we will then approach individuals from the CRGs. There will be no specific tutorials, but the past has shown that the presence of code developers was used by other participants to solve application problems.

6. Budget, expressed in Euro, and how much is being applied for from the ESF Psi-k Programme. In the past, this has been limited to about 9k Euro.

The workshop would be one week long. For 30 particiapants, this would correspond to Number_of_participants * days_of_stay * daily_allowance, or, roughly, 30*5*100 = 15,000 Euros. We need about 1.500 Euros for publication of the contributions in the form of a booklet

We would therefore request 8.000 Euros from Psi-k, and put in a proposal for 7.000 Euros from CECAM. We would also ask other sources for funding, such as the DGK. We also hope to attract funding via the ESF-EuroMinScI program to cover funding for travel for participants.

7. A statement about other organisations which will be applied to for co-sponsorship and additional funding, e.g. any EU Network, CECAM, CCP-9 in the UK, etc.

CECAM, which has generously co-funded our Mineral Physics workshops in the past. ESF in the framework of the EuroMinSci-EUROCORES. Here a funding decision will be taken in September, and the leaders of the collaborative research groups will then be asked to support this workshop.

8. Where it is hoped the workshop would be held.

We wish to continue to hold the workshop at CECAM in Lyon.

9. Plans about inviting and financing any participants from America.

We expect to have three or four US participants. They will be expected to cover their travel expenses, while they will receive the usual daily allowance.