Suggestion for a

EUROCORES

in

European Mineral Sciences Initiative
(EuroMinScI)

The physics and chemistry of minerals with their behaviour studied by integrating experimental and computational methods

0. BACKGROUND

This suggestion for a EUROCORES programme can be traced back to discussions at an ESF workshop held in Rome in September 2001, attended by the chairs of a number of ESF networking activities in the material sciences.

This document has been drafted after a meeting of interested scientists from 10 countries in Frankfurt am Main on 28th October 2003. This meeting mandated a provisional executive committee to formulate the following scientific case for a EUROCORES. This provisional executive committee consists of the following, representing both experimental and computational mineralogy

Prof. Michael Carpenter, Dept. of Earth Sciences, Cambridge.
Prof. Francesco Mauri, Laboratoire de Minéralogie-Cristallographie, Paris.
Prof. Björn Winkler, Institut für Mineralogie, Frankfurt a. M.
Prof. Sandro Scandolo, Abdus Salam ICTP, Trieste

1. SCIENTIFIC SCOPE

1.1 **Integration of mineral physics**

In the last 10 years there have been huge advances in the use of physics-based experimental techniques such as nuclear magnetic resonance spectroscopy, synchrotron radiation, neutron scattering, phonon spectroscopy, laser-ablation based techniques, *etc*. to study mineral properties and behaviour. There have been similar huge advances in atomistic computer simulation. At the same time, it has become possible to make measurements of many properties of minerals *in situ* at extreme conditions of temperature and pressure corresponding to those existing in the earth's interior. A recent prominent example was the experimental and theoretical determination of the temperature at the inner core – outer core boundary and the chemistry of the Earth's core. While many of the techniques have originated within physics, their development owes much to chemists, materials scientists and earth scientists who should be understood as included everywhere in this outline plan.

The new experimental techniques have benefited from the parallel development of computer simulation. What is required now is a managed programme, such as an ESF EUROCORES, to draw together the experimental and computational activities, and the different experimental techniques, into integrated research projects. There is also a need for young researchers from a background in earth sciences to be trained more in the physics-based techniques, where the methods are very different from traditional earth science. Experiment can only observe what happens, usually on a macroscopic or mesoscopic scale, and computer simulation is needed to link the data to conceptual models to achieve understanding at the atomic level and to predict properties and behaviour at extreme conditions which cannot be achieved in the laboratory. Sometimes it calls for separate 'computer experiments' while at other times computer simulation is needed even to interpret the experimental data uniquely. Thermodynamics needs information on non-standard states from simulation. The computer simulations increasingly involve quantum mechanical calculation of all the valence electrons in the system to represent accurately the interatomic bonding.

With the application of modern techniques and the integration of experimental and atomistic modelling approaches, the study of Earth and planetary materials has much to contribute to Geoscience. The proposed EUROCORES is focused on the basic science of minerals. We note, however, that minerals show a fantastic range of diverse and complex structures whose potential for new technological materials has not yet been fully exploited. Also, specific areas of societal needs where mineral scientists are making a significant contribution include the encapsulation of radioactive waste, bio-mineralisation, weathering, pollution, and the use of minerals as templates or models for nanomaterials.

In conclusion, the very rapid scientific advance in recent years has led to the need for a EUROCORES-type of managed programme to promote

- firstly integrated research on minerals using both computer simulation and modern experimental techniques;
- secondly European wide access to and training in the very best experimental and simulation techniques

1.2 **Specific directions of research**

As this EUROCORES is focused on the atomistic understanding of structures, properties and processes of minerals, we envisage that the specific areas of research will include:

a) Behaviour at high pressures and temperatures: The physical properties (including thermoelastic properties) and phase transitions of minerals determine much of the bulk properties and evolution of the deep earth and other planets.
b) Structures and properties of amorphous and disordered materials: This topic includes chemical and structural disorder. Disordered structures generally develop by non-equilibrium processes and have properties which are quite distinct from crystals.
c) Defects and microstructures: Natural crystals are never perfect. They contain defects and microstructures, which substantially modify mechanical, electrical, and transport properties.
d) Transport mechanisms at the atomic length scale: This includes diffusion, defect migration, leaching, thermal and electrical conductivity, with strong links to b) and c) above.

e) Trace elements and isotope partitioning: The partitioning of trace elements between minerals and melts provides quantitative constraints on models of melting in the earth's crust and upper mantle. Isotope ratios in minerals provide much of the data available to earth scientists on geological timescales, sources of fluids or magmas, climate change, meteorite origin and evolution, *etc*.. In biominerals it indicates environmental conditions.
f) Structure, properties and reactivities of mineral surfaces: Interactions of the biosphere, atmosphere and hydrosphere with the lithosphere occur on mineral surfaces. The critical processes are on the atomic length scale and can now be investigated with very high resolution experimentally and theoretically.
g) Spectroscopy of minerals and the quantitative interpretation of spectra: While spectroscopic techniques have been used in the Geosciences for many years, it is only now that recent advances in instrumentation and theory allow a quantitative understanding of the relationship between the atomistic structure and the spectroscopic data.

3. Integration of simulation and experiment

It would be the intention for post-docs and PhD students to spend extended periods in other centres beside their main one in order to be link persons in collaborations and to broaden their experience. It is particularly important for the simulators to be immersed also in an environment of experimentalists.

4 Access to advanced laboratory techniques, computational resources and mature modelling approaches

The highly specialised equipment and the expertise required to conduct state-of-the-art experiments or simulations is only available in a few groups spread around Europe. The EUROCORES programme would facilitate access to advanced laboratory equipment, such as high pressure devices, computational resources, such as clusters, and provide a platform to exchange knowledge about computational and experimental approaches.

5 Networking

More experimentalists and computationalists oriented towards mineralogy are needed. In the past a very small number have been recruited from a background in physics or chemistry, but it will now be necessary to find and train them from the mineralogy community. We propose associating workshops with the main research programme, perhaps using European Marie Curie training sites.

6 European dimension

It is obvious that individual research groups in a single country are not large enough for achieving the goals outlined above. The various items of expensive equipment and the various types of expertise, particularly for computer simulation, are spread between centres in different countries. The need for Europe to act as a unit is even more painfully obvious when one sees Americans working as one community.

European collaboration is important, both for the strong research institutes and for the small groups or isolated researchers, to keep at the world forefront of science. Thus it is envisaged that some projects will involve measurements on the same samples in different laboratories. A EUROCORES programme would give a platform for building collaboration in this field where there is a lack of suitable structures.

There are strong groups active in mineral physics in several European countries (including UK, France, Germany, Italy and Spain) and some first class individual researchers or small groups in other countries including Austria, Norway, Poland, Portugal, Slovak Republic, Sweden and Switzerland.

7 Requirements

The research outlined above requires that in this EUROCORES

- each proposal will be presented by principal investigators of at least two different participating countries
- each proposal contains a clearly identifiable experimental and computational part. One criteria in the assessment of the proposals will be the extent to which these two parts are integrated and, hence, the proposal will explain in detail the complementarity of the experimental and computational part and how synergies will be generated by the collaboration.

We anticipate, that subject to the rules of the national funding agencies, funding will be available for personnel (max. 1 post doctoral worker, or, alternatively, 2 Ph. D students, per principal investigator), travel, consumables and equipment.