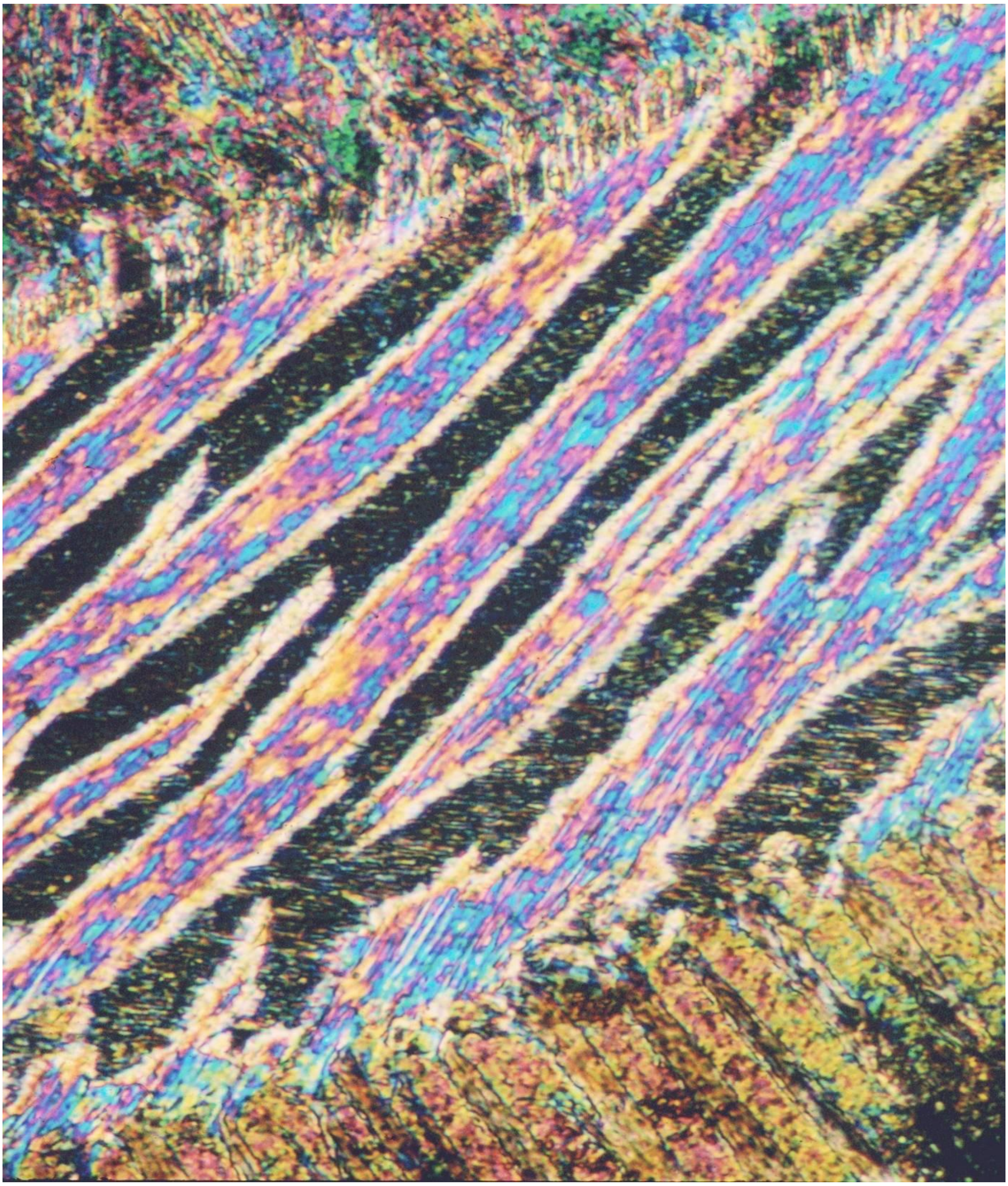
EUROPEAN
SCIENCE
FOUNDATION
SETTING SCIENCE AGENDAS FOR EUROPE

EUROCORES Programme
European Collaborative Research

EuroMinScI
European Mineral Sciences Initiative

FINAL EUROMINSCI CONFERENCE

Valvvf Obernai, France, 24-26 November 2008



European Science Foundation

The European Science Foundation (ESF) was established in 1974 to create a common European platform for cross-border cooperation in all aspects of scientific re-search. With its emphasis on a multidisciplinary and pan-European approach, the Foundation provides the leadership necessary to open new frontiers in European science.

Its activities include providing science policy advice (Science Strategy); stimulating cooperation between researchers and organisations to explore new directions (Science Synergy); and the administration of externally funded programmes (Science Management). These take place in the following areas: Physical and engineering sciences; Medical sciences; Life, earth and environmental sciences; Humanities; Social sciences; Polar; Marine; Space; Radio astronomy frequencies; Nuclear physics. Headquartered in Strasbourg with offices in Brussels, the ESF's membership comprises 75 national funding agencies, re-search performing agencies and academies from 30 European nations. The Foundation's independence allows the ESF to objectively represent the priorities of all these members.

EUROCORES

The aim of the European Collaborative Research (EUROCORES) Scheme is to enable researchers in different European countries to develop collaboration and scientific synergy in areas where European scale and scope are required to reach the critical mass necessary for top class science in a global context.

The scheme provides a flexible framework which allows national basic research funding and performing organisations to join forces to support excellent European research in and across all scientific areas.

Until the end of 2008, scientific coordination and networking is funded through the EC FP6 Programme, under contract no. ERAS-CT-2003-980409. As of 2009, the National Funding Organisations will provide the funding for the scientific coordination and networking in addition to the research funding.

www.esf.org/eurocores

Preface from the EuroMinScI Programme Coordinator

It is our pleasure to welcome you all to the final EuroMinScI Conference in Obernai!

The European Collaborative Research (EUROCORES) Programme EuroMinScI (European Mineral Sciences Initiative, www.esf.org/eurominsci) draws together different experimental techniques and computational activities into integrated research projects. Sometimes it calls for separate ‘computer experiments’ while at other times computer simulation is needed even to interpret the experimental data uniquely. It also addresses the need for young researchers with an academic background in earth sciences to be trained more in the physics-based techniques, where the methods are very different from traditional earth sciences. A “bottom-up” approach is adopted, in which participating scientists propose their own research projects within the broad context of EuroMinScI Programme.

The annual EuroMinScI Conference is the major event for the EuroMinScI scientific community to present its latest activities and key achievements within this Programme. It allows all partners in the programme to meet over an extended period to discuss their projects, as well as to exchange with scientists from other CRPs and, very important, establish links outside the EuroMinScI community. We hope that this last EuroMinScI conference will be as pleasant and fruitful as its predecessors, and that it will further enhance the strong potential of the EuroMinScI Programme to put European Science at the competitive leading edge in terms of modern mineralogy.

On behalf of the European Science Foundation and the EuroMinScI funding agencies, we wish to thank Björn Winkler who helped developing the attractive programme of this final conference.

October 2008, Strasbourg

Kai Rankenburg

EuroMinScI Programme Coordinator

Anne-Sophie Gablin / Anne Garel

EuroMinScI Administrators

The EuroMinScI Programme is financed by funding agencies from 12 European countries: FWF, Austria; FWO, Belgium; FNRS, Belgium; GA-CR, Czech Republic; EstSF, Estonia; CNRS, France; DFG, Germany; MTA, Hungary; CNR, Italy; SAV, Slovak Republic; MEC, Spain; VR, Sweden; NERC, United Kingdom, and by the European Science Foundation (ESF) under the EUROCORES Programmes, with support by the European Commission, DG Research (Sixth Framework programme, contract ERAS-CT-2003-980409).

Preface from the Chair of the EuroMinScI Steering Committee

The networking activities of the ESF EUROCORES “European Mineral Science Initiative”, EuroMinScI, are now coming to an end with this conference. As individual projects within the collaborative research projects, CRPs, started at different times, some projects still will continue to run for up to a year. Hence, the total scientific output of EuroMinScI cannot be evaluated yet. However, it is already clear now that the major aims of this EUROCORES have been achieved. When we proposed this European collaboration, we wanted to establish a network aimed at producing outstanding science in the field of mineral physics. Clearly, the numerous publications in high impact journals unambiguously give evidence of the excellent science that has been done within the EuroMinScI CRPs. The second aim of EuroMinScI was to stimulate collaborations in which simulations and experiments complemented each other. This aim also has been achieved, as can be seen from the many publications which rely on both experimental and simulation data. Finally, we wanted to provide opportunities to disseminate state-of-the-art experimental and theoretical approaches within the mineral physics community and related neighbouring scientific disciplines. The ESF contributed generously to numerous EuroMinScI-related networking activities, and thereby provided opportunities to present recent advances in mineral physics achieved within EuroMinScI to an extended scientific community. The EuroMinScI collaboration also had an impact beyond the current activities. The network was, for example, instrumental in convincing funding authorities to provide funding for the “extreme conditions” diffraction station at a new synchrotron at Desy in Hamburg – without the contributions of the EuroMinScI community, this development would very likely not have happened.

In the initial stages of this EUROCORES it was planned to have a prolongation after the first funding period in order to be able to fully exploit the progress made in the first three years. Regrettably, it has not been possible to secure the required funding. However, as I have heard from a number of participants, EuroMinScI is seen as such a successful enterprise that there are now a number of groups who are planning proposals for new EUROCORES. I very much hope that these proposals are successful and that there will be further European networks dedicated to research in mineral physics – I think EuroMinScI has demonstrated that such a framework is efficient and necessary to remain competitive.

I would like to thank all participants for their efforts and I hope that everybody enjoyed the meetings as much as I did. I would also like to thank Anne-Sophie Gablin, Bernard Avril, and Kai Rankenburg for their commitment, support and understanding – without them, this EUROCORES would not have been as successful as it was.

Frankfurt 1/11/2008

Bjoern Winkler

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PROGRAMME

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PROGRAMME

On line at http://www.esf.org/eurominsci

Sunday 23 November 2008

16.00	Registration at the hotel and at ESF desk
19.00	Welcome drink
20.00	Dinner

Monday 24 November 2008

08.30	**Conference Opening** **Kai Rankenburg** (EUROCORES Programme Coordinator, ESF)

CRP1 - Calcareous Biocrystals (BioCalc)

09.00	**Jean-Pierre Cuif** (CNRS Université de Paris XI, Faculté des Sciences, Département de Géologie, France) *Microstructure and Mineral Behaviour : Investigating the specific patterns of the Ca-carbonate crystals produced by living organisms, from microstructural to molecular scale*
09.45	**Alberto Perez-Huerta** (University of Glasgow, Department of Geographical & Earth Sciences, United Kingdom) *Crystallography of calcite crystals in pearls*
10.05	**Maggie Cusak** (University of Glasgow, Department of Geographical & Earth Sciences, United Kingdom) *Oxygen isotope equilibrium in brachiopod shells in the context of biological control*

10.30	Coffee break

CRP2 - The rheology of the subducting slab and mantle (euroSLAB)

11.00	**David Dobson** (University College London, United Kingdom) *Mineral Physics and Chemistry of the Earth : The rheology of the slab and mantle from experiment and simulation*
11.45	**Arnaud Metsue** (CNRS Université des Sciences et Technologies de Lille, France) *Mineral Physics and Chemistry of the Earth : A new description of the 3D dislocation core structure of forsterite by coupling Peierls-Nabarro and element-free Galerkin methods*
12.05	Lunch

CRP 3 - Mineralogy and Chemistry of Earth's core (MCEC)

13.15	**Igor Abrikosov** (Linköping University, Sweden) *Elements and Alloys at Extreme Conditions : Ab initio theory of Fe-Ni alloys at Earth's core conditions*
14.00	**Segej Simak** (Linköping University, Department of Theoretical Physics, IFM, Sweden) *Elements and Alloys at Extreme Conditions : Theory of alloys under high pressure and temperature: a supercell technique*

CRP4 - Ordering of Ions in Minerals (ORION)

14.20	**Alberto Garcia** (Institut de Ciencia de Materials de Barcelona, Spain) *Overview of results of the ORION project*
15.05	Coffee break
15.30	**Javier Lopez Solano** (Universidad del País Vasco, Facultad de Ciencia y Tecnología, Departamento de Física de la Materia Condensada, Bilbao, Spain) *Atomistic Understanding of Minerals : A model hamiltonian to study ionic conductivity in sodium nepheline*
15.50	**Ramona Langner** (Ruhr-Universität Bochum, Institut für Geologie, Mineralogie und Geophysik, Germany) *Ordering of the Al Cation Distribution in the Octahedral Sheets Related to the Ordering of Al in the Tetrahedral Sheets of Phlogopite Investigated by 2D CPMAS NMR and Monte Carlo Simulations*
16.10	**Predrag Vulic** (Universität Innsbruck, Institut für Mineralogie und Petrographie, Austria) *Defects and Disorder in Minerals : On the existence of satellite reflections in natural nephelines*
16.30	**Poster session**
20.00	Dinner

Tuesday 25 November 2008

CRP7 - Hydrogen in Minerals (HydroMin)

09.00 **Bjoern Winkler** (Johann Wolfgang Goethe-Universität Frankfurt, Institut für Geowissenschaften, Abteilung Kristallographie, Germany)
Microstructure and Mineral Behaviour : The HydroMin-project

09.20 **Kate Wright** (Curtin University of Technology, Nanochemistry Research Institute, Department of Applied Chemistry, Perth, Australia)

Microstructure and Mineral Behaviour: Defects and deformation in olivine: from molecules to mantle

09.40 **Etienne Balan** (Institut de Recherche pour le Développement, Université Paris VI, Institut de Minéralogie et Physique des Milieux Condensés, Paris, France)

Atomistic Understanding of Minerals: Theoretical study of the infrared absorption spectra of OH groups in minerals

10.00 **Keith Refson** (Rutherford Appleton Laboratory, Chilton, United Kingdom)

Microstructure and Mineral Behaviour : First-principles simulation of spectroscopy in minerals under pressure

10.30 Coffee Break

11.00 **Simon Delattre** (Institut de Recherche pour le Développement University Paris VI, Institut de Minéralogie et Physique des Milieux Condensés, France)

First principles modeling of the IR spectrum of a natural nanotube: imogolite Al2O3(OH)3SiOH

11.20 **Jannick Ingrin** (Université Paul Sabatier, Laboratoire des Mécanismes et Transferts en Géologie, Toulouse, France)

Microstructure and Mineral Behaviour : Hydrogen diffusion in apatite measured from H-D exchange experiments

11.40 **Marc Blanchard** (CNRS Université Paris VI, Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC) Département de Mineralogie, France)

Defects and Disorder in Minerals : Incorporation of water in iron-free ringwoodite: a first-principles study

12.00 Lunch

CRP 5 - Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

13.15 **Richard Harrison** (University of Cambridge, Department of Earth Sciences, United Kingdom)

A presentation of the MICRPOMAGN CRP

14.00 **Maike Luebbe** (Ludwig-Maximilians-Universität München, Department für Geo- und Umweltwissenschaften, Germany)

Microstructure and Mineral Behaviour: Magnetic Properties of Fe2O3-Ti1-xO-Fe2O3 and Fe2O3-FeTiO3-Fe2O3 Sandwich Structures

CRP6 - Subgrain structure development in rocks and metals (MINSUBSTRDYN)

14.20	**Sandra Piazolo** (Stockholm University, Department of Geology and Geochemistry, Sweden) *Microstructure and Mineral Behaviour: Substructure dynamics in minerals and metals: New insights from experiments and numerical simulations*
15.05	**Joyce Schmartz** (RWTH Aachen University) *Microstructure and Mineral Behaviour : On the Kinetics of Fluid Inclusions in Recrystallizing Rocks*
15.25	Coffee Break
16.00-19.30	**Wrap-up meeting of Project Leaders, Review Panel and Management Committee Members**
20.00	Official Conference Dinner

Wednesday 26 November 2008

Mixed Session

09.00	**Gernot Nehrke** (Alfred-Wegener Institut für Polar- und Meeresforschung, Germany) *Biomineralizationprozesses in foraminifera* **Andrzej Grzechnik** (University of the Basque Country, Faculty of Sciences and Technology, Department of Condensed Matter Physics, Bilbao, Spain) *Atomistic Understanding of Minerals : Single-crystal and powder x-ray diffraction measurements on single-crystal diffractometers with area-sensitive detectors at high pressures* **Lars Olsen** (University of Copenhagen, Faculty of Science, Department of Geography and Geology, Denmark) *Atomistic Understanding of Minerals : Influence of pressure and coordination environment on bonding in bismuth sulphides: An ab initio study on Bi2S3 and Cu4Bi5S10* **Nathan Church** (University of Cambridge, Faculty of Physical Sciences, Department of Earth Sciences, UK) *Microstructure and Mineral Behaviour : Electron holography of oxy-exsolution microstructures in synthetic titanomagnetites*
10.30	Coffee break
12.00	**Lunch**
13.00	**Group discussions**
15.00	Wine Tasting
20.00	Dinner

Thursday 27 November 2008

08.45 Departure (after breakfast)

All posters will be on display during the whole duration of the conference

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LIST OF ABSTRACTS

CONFERENCE ABSTRACTS - TALKS

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Project
05_EMINS_FP08_MCEC / Mineralogy and Chemistry of Earth's core (MCEC)

Elements and Alloys at Extreme Conditions

Ab initio theory of Fe-Ni alloys at Earth’s core conditions

I. A. Abrikosov1 , A. S. Mikhaylushkin1, C. Asker1 , M. Ekholm1 , U. Kargen1 , S. I. Simak1 , N. Dubrovinskaia2, L. Dubrovinsky3
1Department of Physics, Chemistry and Biology, Linköping University, Sweden, 2 Mineralogical Institute, Heidelberg University, Heidelberg, Germany, 3 Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany

We review recent progress in theoretical description of Fe-Ni alloys at extreme conditions. We show that at temperature of 5000-6000 K and pressure of 350 GPa three close-packed phases, hcp, bcc, and fcc, are very close in energy to each other, and the energetic balance between them depends sensitively on the nature and amount of alloying elements [1,2]. We emphasize the importance of a proper treatment of magnetic effects. We discuss a degree of disorder which is present in the alloy at the above conditions, as well as the nature and range of interatomic interactions in Fe-Ni system. Finally, anomalous elastic properties of Fe-Ni alloys will be discussed.

[1] L. Dubrovinsky, N. Dubrovinskaia, O.Narygina, A. Kuznetzov, V. Prakapenka, L. Vitos, B. Johansson, A. S. Mikhaylushkin, S. I. Simak, and I. A. Abrikosov, “Experimental Evidences for Body-Centred-Cubic Phase of Iron-Nickel Alloy in the Earth’s Core”, Science 316, 1880 (2007).

[2] A. Mikhailushkin, S. I. Simak, L. S. Dubrovinsky, N. A. Dubrovinskaia, B, Johansson, and I. A. Abrikosov, "Pure iron compressed and heated to extreme conditions", Phys. Rev. Lett. 99, 165505 (2007).

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Atomistic Understanding of Minerals

Theoretical study of the infrared absorption spectra of OH groups in minerals

E tienne Balan (1), Keith Refson (2) Marc Blanchard (1), Simon Delattre (1), Michele Lazzeri (1), Merlin Méheut (1), Jannick Ingrin (3), Francesco Mauri (1), Kate Wright (4), Bjoern Winklkler (5)
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The infrared absorption bands related to the stretching vibrational modes of OH groups are widely used in mineralogy, either to probe the structure of hydrous minerals or to investigate the speciation and concentration of dissociated water in nominally anhydrous minerals. However, the interpretation and use of the measured absorption bands is often a matter of debate, even in ordered and chemically pure samples. Recent theoretical developments make it possible to establish unambiguous relationships between the IR spectrum and the microscopic (crystallographic) structure of minerals. This is done by computing the low-frequency dielectric tensor of the crystal, within the framework of density functional theory, and combining it with an electrostatic model taking into account the experimental geometry and the sample microstructure. Applications of this approach to the quantification of OH defects in nominally anhydrous minerals (Balan et al. 2008a) and the interpretation of the spectrum of low-temperature hydrous minerals (Balan et al. 2007, 2008b) will be presented.

References:

Balan E., Refson K., Blanchard M., Delattre S., Lazzeri M., Ingrin J., Mauri F., Wright K., Winkler B. (2008a) Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 93, 950-953. abstract

Balan E., Blanchard M., Hochepied J.-F., Lazzeri M. (2008b) Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. Physics and Chemistry of Minerals, 35, 279-285. abstract

Balan E., Lazzeri M., Delattre S., Meheut M., Refson K., Winkler B. (2007) Anharmonicity of inner-OH stretching modes in hydrous phyllosilicates: Assessment from first-principles frozen-phonon calculations Physics and Chemistry of Minerals, 34, 621-625.

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Defects and Disorder in Minerals

Incorporation of water in iron-free ringwoodite: a first-principles study

Marc Blanchard (1), Etienne Balan (1,2) and Kate Wright (3)
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Ringwoodite (gamma-Mg2SiO4), one of the main minerals of the transition zone, can incorporate a significant amount of water in the form of OH within its crystal structure (up to ~2.7 wt% H2O). The presence of water affects the physical and chemical properties of ringwoodite (e.g. electrical conductivity, seismic velocities) and therefore has important implications for the dynamics of the transition zone.

In the present study, we perform first-principles calculations based on density functional theory to derive the structures, infrared active OH stretching modes and relative energies of OH-defects in ringwoodite. Two types of fully protonated cationic defects in normal spinel were considered at 0 and 20 GPa, i.e. [VMg(OH)2]x, [VSi(OH)4]x defects. In addition, two defects associated with the partial inversion of the spinel structure have been investigated. The infrared spectrum and evolution with pressure of these OH-defects make it possible to interpret the major IR absorption bands experimentally observed. The main absorption band at ~3150 cm-1 corresponds to protons located between the O-O pairs shared by 16c and 16d octahedra, instead of OH along the tetrahedral edges as usually proposed in the literature. The large width of this band is most likely related to the association of OH defects with the various cationic configurations related to the partial inversion of a vacancy-bearing spinel structure. The less intense band at ~3675 cm-1 is assigned to hydrogarnet-type defects with a protonation of the tetrahedral edges. These results emphasize the importance of taking into account the structural relaxation undergone by defects, instead of using empirical correlation, to assign OH stretching bands to specific O-O pairs of the structure.

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Project
05_EMINS_FP13_MICROMAGN / Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

Topic: Microstructure and Mineral Behaviour

Electron holography of oxy-exsolution microstructures in synthetic titanomagnetites

Nathan Church, Richard Harrison, Takeshi Kasama, Rafal Dunin-Borkowski
Department of Earth Sciences, Cambridge, UK; Centre for Electron Nanoscopy, Kongens Lyngby, DK

Intergrowths of titanomagnetite and titanohematite or ulvospinel resulting from oxy-exsolution or spinodal decomposition are regularly observed in paleomagnetic specimens. This microstructure is thought to be responsible for anomalous paleointensity measurements of historic lavas and experiments have shown that bulk magnetic properties are dramatically affected by the creation of these structures. However, previous studies have not been able to rigorously measure the effects of the geometry and composition of the magnetic phases. Electron holography, a TEM technique that allows the quantitative measurement of the magnetic flux at a nanometer scale, provides an opportunity to investigate how these variables influence magnetostatic interactions and inform our interpretation of magnetic data from rock samples showing these textures.

The samples used in this study are synthetic polycrystalline spinels with compositions spanning the magnetite-ulvospinel solid solution, which were re-sintered under oxidizing conditions to create oxy-exsolution structures of paramagnetic titanohematite lamellae separating blocks of ferrimagnetic titanomagnetite. The composition of the titanomagnetite is governed by the starting material and oxygen fugacity during the re-sintering process; using the appropriate conditions we were able to exsolve samples with compositions approaching pure magnetite, and the size of the ferrimagnetic particles are pseudo-single-domain to multidomain. Electron holography was carried out on thinned samples to measure the magnetic flux between these interacting particles. Measurements of these magnetostatic interactions will inform micromagnetic models of interacting pseudo-single-domain particles, and future work will allow us to more carefully control the width of the paramagnetic lamellae and hence inter-particle spacing to accurately interpret the effect of these microstructures on the properties of natural paleomagnetic samples.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

Microstructure and Mineral Behaviour

The BioCalc project: investigating the specific patterns of the Ca-carbonate crystals produced by living organisms, from microstructural to molecular scale

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During this three-year project, substantial progress has been made regarding the crystallisation process leading to formation of the Ca-carbonate units produced by many groups of Invertebrates. Investigation was primarily based on two models: the calcite prisms of the mollusk shells and the aragonite fibres of coral skeletons. As shown by current literature (e.g. Veis, Science 2005, v.307, p. 1419 or Williams, Geol. Soc. London 2008, spec. paper n° 303), it is commonly admitted that these two types of calcareous materials result from distinct crystallization mechanisms: i) crystallization driven by specifically secreted biochemical compounds (matrices of mollusc prisms) or ii) crystallization induced by biological activity with low control of size, shape and three-dimensional arrangement of crystals (corals). In this case “crystals adopt sizes, shapes and spatial arrangements comparable to purely chemical precipitations” (Veis, 2005). Results of the BioCalc project fully disprove this concept.

Result 1: In both mollusk and corals, crystallization occurs under close and permanent control by biochemical compounds, the compositions of which are taxonomy dependant. Both are “matrix mediated structures”, following the Lowenstam terminology (1981). The growth units are not the long described crystal-like materials (e.g. prisms) but a few micron-thick growth-layer, common to most types of microstructures.

Result 2: In all the investigated calcareous structures, growth layers are built by densely packed sub-micrometric spheroidal units. Their dimensions (in the x10 nanometer range) and the location of organic material irregularly coating the mineral phase, explain why synchrotron based maps carried out at micrometric resolution always reveal a striking correspondence between mineral layering and distribution of organic components. This nano-structure is a key point to understand the specific crystallization process of the calcareous biocrystals.

Result 3: Transmission electron microscopy has shown that within a growth layer crystallization occurs as a final step. Ca-carbonate is transported from the mineralizing cells to the external space not as free ions but as amorphous material associated to the glyco-protein components that built the spheroidal units. Crystallization occurs by disruption of the association between Ca-carbonate molecules and the organic Ca-carbonate conveyor. The Ca-carbonate crystalline lattice is then formed, but not as a compact crystal with typical crystalline growth faces. In biocrystals, crystallization never produces faceted crystals. At the nanometer scale, the organic material that has initially carried the Ca-carbonate molecules is pushed away from the

	crystal lattice in formation, resulting in the reticulate structure at the nanoscale, typical for biocrystals. Presence of “normal“ growth surface in biogenic Ca-carbonates is always due to failure of the biological control. Result 4: Thus, in contrast to the geochemical model, crystallization of Ca-biocarbonates does not occurs as a freely running process, allowing the common chemical rules of crystallization to be applied. Crystallization occurs within the glyco-protein hydrogel that results from the first step in the formation of the growth layer. As a major consequence, microprobe and SIMS measurements have repeatedly shown that in a given organism, the different microstructural domains of the skeletons exhibit specific minor element concentrations or isotopic fractionations. This “vital effect” predicted in the Urey’s paper (1951) is thus understandable on the basis of the two step model of biocrystallization.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

Microstructure and Mineral Behaviour

Oxygen isotope equilibrium in brachiopod shells in the context of biological control

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With their long geological history and stable low magnesium calcite, Rhynchonelliform brachiopods are attractive sources of environmental data such as past seawater temperature (Auclair et al., 2003; Brand et al., 2003; Buening and Spero, 1996; Parkinson et al., 2005). The outer primary layer of acicular calcite is isotopically light in both δ18O and δ13C while the secondary layer calcite fibres are in oxygen isotope equilibrium with ambient seawater (Parkinson et al., 2005). The calcite fibres of the secondary layer are parallel to the shell exterior. Electron backscatter diffraction (EBSD) reveals that the fibres are effectively single crystals with the calcite c-axis perpendicular to the fibre axis (Cusack et al., 2007; Pérez-Huerta et al., 2007; Schmahl et al., 2004). The granular nature of the fibres is evident in Atomic Force Microscopy (AFM) where the addition of bands of calcite granules to the growing fibre is clear (Cusack et al., 2008). These bands of granules are thus added over the duration of fibre growth with crystallographic orientation being maintained throughout. Although there remains much to be understood about how this precise biological control is achieved, the attainment of isotope equilibrium under such strict biological influence is counter-intuitive.

Auclair, A.-C., et al., 2003 - Chemical Geology. 202, 59-78. Brand, U. et al. 2003 - Chemical Geology.198, 305-334. Buening, N., Spero, H.J.1996 - Marine Biology, 127, 105-114. Cusack, M. et al. 2007 - CrystEngComm, 9, 1215-1218. Cusack, M. et al. 2008 - J. Structural Biology, 164, 96-100.Parkinson, D. et al. 2005 - Chemical Geology, 219,193-235. Pérez-Huerta, A. et al. 2007 - Journal of The Royal Society Interface, 4, 33-39. Schmahl, W.W. et al. 2004 - European Journal of Mineralogy, 16, 693-697.

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Project
05_EMINS_FP21_HYDROMIN / Hydrogen in Minerals (HydroMin)

Atomistic Understanding of Minerals

First principles modeling of the IR spectrum of a natural nanotube: imogolite $Al_2O_3(OH)_3SiOH$

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Although the presence of aluminosilicated gels in soils influences markedly their properties, the structure of these short-range ordered species remains poorly constrained. From similarities of IR patterns, imogolite ($Al_2O_3(OH)_3SiOH$) a natural medium-range ordered nanotube-based material has been proposed as a structural model for a class of gels with an Al/Si ratio close to two. However, the absence of long-range order in imogolite has hampered a refinement of its structure using classical diffraction techniques. For this reason, the structure has been largely determined from transmission electron microscopy and an empirical interpretation of its infrared spectrum. To support the assignment of absorption bands to specific structural units, an ab-initio study of the vibrational properties of imogolite was undertaken. Indeed, theoretical methods now enable the accurate computation of infrared spectra, and more generally of vibrational properties, from crystal structures (e.g. Blanchard et al. 2008, Balan et al. 2008, Méheut et al. 2007).

In the case of imogolite, an approach based on the curvature of a continuous dielectric medium, as previousy used to model the IR spectrum of chrysotile nanotubes, was not adapted because the material is constituted of single-wall nanotubes. In that case, structural relaxations are expected to be more important and calculations were performed by explicitely considering the atomic-scale structure of the tubes within the Density Functional Theory framework using the Generalized Gradient Approximation as implemented in the SIESTA code. The low-frequency dielectric tensor of isolated tubes has been computed from the ab initio Born effective charge tensors and vibrational modes. The infrared spectrum of imogolite was then computed for various aggregation states of nano-tubular particles using classical electrostatic laws. The comparison with experimental spectra makes it possible to unambiguously assign the observed bands and to determine the spectral changes related to a variation in the diameter of the tubes. Beside a more accurate approach of the details of the crystal structure, these results should improve the identification of such disordered phases in complex soil samples.

Balan E., Refson K., Blanchard M., Delattre S., Lazzeri M., Ingrin J., Mauri F., Wright K., Winkler B. (2008) Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 93, 950-953.

Blanchard M., Lazzeri M., Mauri F., Balan E. (2008) First-principles calculation of the infrared spectrum of hematite. American

	Mineralogist, 93, 1019-1027. Meheut M., Lazzeri M., Balan E., Mauri F. (2007) Equilibrium isotopic fractionation between kaolinite, quartz and water: prediction from first-principles density-functional theory. Geochimica et Cosmochimica Acta, 71, 3170-3181.

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Project
05_EMINS_FP04_CUBCAT / Reactivity of (Fe,Ni)S minerals and cubane clusters with gas and amino-acids: towards an understanding of the emergence of life (CUBCAT)

Reactivity & Structure of Surfaces & Interfaces

The Iron Sulphide Greigite

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Natural biological systems are capable of fixing environmental CO2 under moderate conditions, suggesting the great potential of bio-inspired catalysts in future carbon-activation technologies. Investigations into the surfaces of the iron sulphide minerals mackinawite (FeS) and greigite (Fe3S4) have shown them to be structurally similar to (Ni, Fe)S cubane cluster molecules implicated in the formation of proto-metabolism, the pre-cursor to life. Bio-catalysts with the (Fe,Ni)S cubane-cluster structure metabolise such volatile molecules as H2, CO and CO2, and the design and development of a synthetic catalyst based upon these molecules would be a major achievement.

The absence of theoretical treatments of greigite has held back the understanding of this important mineral. The success of the GGA+U method in the description of both iron oxides and sulphides demonstrate the power of the technique, and its application to the greigite bulk structure has confirmed the magnetic and structural behaviour of this spinel, with the absence of any transition to a monoclinic structure at low temperature. The agreement with experiment is shown to be excellent, and extension to the most important surfaces is discussed.

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Project
05_EMINS_FP07_EuroSLAB / The rheology of the subducting slab and mantle (euroSLAB)

Mineral Physics and Chemistry of the Earth

The rheology of the slab and mantle from experiment and simulation

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We present results of experimental and numerical simulations studies opf rheology of mantle materials or relavence to subducting slab environments.

Upper mantle experiments include lowT-rheology of olivine and garnet and of multi-phase aggregates. During the course of the project the post-perovskite phase of MgSiO3 has been proven to be increasingly important for the D'' region of the lower mantle. Therefore we focussed our xperiments and simulations on this phase, with some important results:

1) We have concluded that CaRiO3 is a good mechanical analogue to MgSiO3.

2) Experiments have shown the reason for the discrepancy between early texture development studies.

3) Post-perovskite is significantly weaker than perovskite in in situ experiments

Recent ab intio simulations of diffusion in the majore lower-mantle mantle phases allow us to predict rheology based on diffusion-controlled deformation mechanisms: these are in excellent agreement with the experiments.

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

not applicable

Overview of results of the ORION project

The ORION CRP
ORION

I will provide an overview of the main results of the ORION (Ordering of Ions in Minerals) project.

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Topic: Atomistic Understanding of Minerals

Single-crystal and powder x-ray diffraction measurements on single-crystal diffractometers with area-sensitive detectors at high pressures

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Modern single-crystal x-ray diffractometers equipped with area-sensitive detectors could easily be used for single-crystal and powder studies at high pressures both at home laboratories and at synchrotron facilities. In this contribution, we will review our own experience with the diffractometers with image plates (IPDS/Stoe) and with the CCD detectors (MAR) . The examples will include the work at our high-pressure laboratory in Bilbao and at the synchrotrons ANKA (Karlsruhe) and HASYLAB (Hamburg). We will also present our approach to single-crystal data indexing, integrating, and correcting for absorption.

Richard Harrison no address **Project** 05_EMINS_FP13_MICROMAGN / Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)	*Microstructure and Mineral Behaviour* A presentation of the MICRPOMAGN CRP

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Microstructure and Mineral Behaviour

Hydrogen diffusion in apatite measured from H-D exchange experiments

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H, Cl and F content in apatite is a strong function of melts composition and is widely used to estimate halogen and water fugacities of magmas. However, the reliability of measurements is highly dependent on the diffusion rate of these species in apatite.

We performed isotope diffusion exchange experiments (H-D exchange experiments) between 973 and 1173K, in a natural apatite gem single crystal from Durango (Mexico; Ca5(PO4)3(F0.91, Cl0.06, OH0.03). The results show that diffusion is highly anisotropic with diffusion fifty times faster parallel to the basal plane than perpendicular to it. The isotopic diffusion rate along the basal plane is defined by the diffusion law: Dbasal = D0 exp[-138 kJmol-1/RT] with D0 equal to 6.7 10-9 m2s-1. This law is much faster than the diffusion laws deduced from exchange experiments between OH, Cl and F (Brenan, 1994); except along the direction [001] for which the rates of isotopic diffusion and exchange are similar. The anisotropy of diffusion of OH-Cl-F species is completely different with diffusion along [001] faster than diffusion along the basal plane.

Our results have direct applications for the interpretation of H/D measurements in apatite from igneous rocks and meteorites.

Brenan J. (1994) Chemical Geology, 110, 195-210

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Defects and Disorder in Minerals

Ordering of the Al Cation Distribution in the Octahedral Sheets Related to the Ordering of Al in the Tetrahedral Sheets of Phlogopite Investigated by 2D CPMAS NMR and Monte Carlo Simulations

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This work is part of the ORION-project (Ordering of Ions in Minerals) within the EuroMinScI programme of the ESF which aims at the elucidation of ionic ordering by combining experimental investigations and theoretical calculations. Previous NMR solid state experiments in phlogopite, a trioctahedral 2:1 layer silicate, indicated a non-statistical distribution of cations and anions in the octahedral sheets: F prefers sites coordinated by three Mg, whereas OH prefers sites with Al as next-nearest-neighbours (Fechtelkord et al. 2003). Further investigations were carried out on phlogopites with various Al-contents and synthesized at different temperatures. Cross-polarization (CP) {1H} 29Si CPMAS NMR experiments were performed to clarify whether the degree of ordering in the octahedral sheets is related to that in the tetrahedral layers. These experiments clearly indicate a direct neighbourhood of aluminium in the tetrahedral sheets to aluminium in the octahedral sheets and, thus, a relationship between the ordering of ions in both sheets.

Support for these conclusions comes also from atomistic simulations of ordering using the so-called ”J formalism” in which total-energy calculations with interatomic potentials are used to generate a set of pair interaction parameters which are then employed in Monte Carlo (MC) simulations (Bosenick et al. 2001, Warren et al. 2001). In phlogopite we have considered the OH-rich extreme, and performed MC simulations for several overall concentrations of Al in the range $0 < x < 1$, finding significant segregation of the Al atoms with a strong spatial correlation between the Al-rich domains in the two layers.

This presentation is supported by the European Science Foundation (ESF) under the EUROCORES programme EuroMinScI (www.esf.org/eurominsci), through contact No. ERAS-CT-2003-980409 of the European Commission, DG Research, FP6, and by the Deutsche Forschungsgemeinschaft (DFG) under project No. Fe486/6-1.

References

Bosenick A, Dove MT, Myers ER, Palin EJ, Sainz-Diaz CI, Guiton B, Warren MC, Craig MS, Redfern SAT (2001) Computational methods for the study of energies of cation distributions: Applications to cation-ordering, phase transitions and solid solutions. Mineral Mag 65: 193-219.

	Fechtelkord, M, Behrens, H, Holtz, F, Fyfe, CA, Groat, LA, Raudsepp, M (2003) Influence of F content on the composition of Al-rich synthetic phlogopite: Part I. New information on structure and phase-formation from 29Si, 1H, and 19F MAS NMR spectroscopies. Am Miner 88: 47-53 Warren MC, Dove MT, Myers R, Bosenick A, Palin EJ, Sainz-Diaz CI, Guiton BS, Redfern SAT (2001) Monte Carlo methods for the study of cation ordering in minerals. Mineral Mag 65: 221-248

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Atomistic Understanding of Minerals

A model hamiltonian to study ionic conductivity in sodium nepheline

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According to previous experimental studies, sodium nepheline is almost a one dimensional ionic conductor [1], with the Na ions moving along rather rigid hexagonal channels formed by an AlSiO_4 framework [2]. The ionic conductivity presents a strong dependence on the Na density, which may be an indication of the existence of two different charge transport mechanisms [1].

We present details of a model hamiltonian which allows for a fast evaluation of macroscopic propierties such as the ionic conductivity, while retaining the main features of the system. The complex many body interactions of the Na ions inside the channel are expressed as just two simple terms, one for the interaction between the Na ions and the channel, and another for the interaction between the Na ions themselves. All the parameters of this model can be fitted from ab initio calculations. A good agreement between results obtained using the present model and the Siesta ab initio code [3] is found for a single-ion-hopping charge transport mechanism.

Using this model hamiltonian to perform molecular dynamics simulations, further understanding of the microscopic origin of the ionic conductivity in sodium nepheline can be obtained in an efficient way.

References:

[1] G. Roth, and H. Böhm, Solid State Ionics 18 & 19, 553 (1986)

[2] M. Gregorkiewitz, Bull. Minéral 107, 499 (1984)

[3] J.M. Soler, E. Artacho, J. Gale, A. García, J. Junquera, and P. Ordejón, J. Phys.: Condens. Matter 14, 2745 (2002)

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Project
05_EMINS_FP13_MICROMAGN /
Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

Microstructure and Mineral Behaviour

Magnetic Properties of Fe2O3-Ti1-xO-Fe2O3 and Fe2O3-FeTiO3-Fe2O3 Sandwich Structures

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At room temperature hematite, Fe2O3, is a canted atiferromagnet and ilmenite, FeTiO3 is a paramagnet. Nevertheless, hematite-ilmenite intergrowths show astonishing high natural remanent magnetism. The magnetic properties of these Fe2O3-FeTiO3 intergrowths must be related to the interface and are described by the “lamellar magnetism hypothesis” (see e.g. [1],[2]).

In order to investigate the magnetic properties of the hematite-ilmenite interface we have grown Fe2O3-Ti(1-x)O- Fe2O3 and Fe2O3-FeTiO3-Fe2O3 structures as well as Fe2O3 thin films on Al2O3(0001). Experiments were also performed with thin films and layered structures grown on Ag(111). The magnetic properties of thin films and sandwich structures grown on the same substrate material were compared. These results can help to illuminate the unusual magnetism of the hematite-ilmenite interface.

On Al2O3(0001) the Fe2O3-Ti(1-x)O- Fe2O3 and Fe2O3-FeTiO3-Fe2O3 sandwich structures differ from the Fe2O3 thin films in their magnetic properties. Although the details of the magnetic properties strongly depend on the growth conditions of the thin films – as the morphology does [3] – a general trend is obvious: If a Ti-bearing interface is included in the thin film the saturation magnetisation is increased by a factor of 1.5 – 2 compared to a thin film without Ti prepared with otherwise same conditions. A large exchange bias, H(eb) ≥ 1 T, was found in natural mineral intergrowths (FeTiO3-bearing Fe2O3). [4] We were not able to confirm an exchange bias effect with our synthetic structures although very thin structures with a single interface showed a small exchange bias of H(eb) ≈ -3 mT which is affected by training and drops to H(eb) ≈ -1 mT after some hysteresis cycles. For thicker layers no H(eb) was found.

The magnetic properties of the Fe2O3-Ti(1-x)O- Fe2O3 sandwich structure on Ag(111) differ in two important aspects from that of the Fe2O3 thin film on Ag(111) at room temperature. First, the remanent magnetic moment acquired at 100 mT is ten times larger than the corresponding value for the Fe2O3 thin film, although the number of hematite layers has only doubled. This difference in remanence intensity points to an intrinsically stronger magnetism of the sandwich structure, most likely due to the intercalated Ti(1-x)O-layer. Secondly, the remanence curves for the sandwich structure are not monotonic, but show an abrupt loss of remanence by some 50 % as the field

	strength is increased above B(flip)=200 mT. Although the details are not all clarified, we can conclude that the Ti-bearing interface in Fe_2O_3-$FeTiO_3$ intergrowths indeed causes the high magnetisation. This is supporting the “lamellar magnetism hypothesis”. [1] P. Robinson et al., Am. Min. 89, 725 (2004) [2] P. Robinson et al., Am. Min. 91, 67 (2006) [3] M. Lübbe et al., in preparation [4] S. McEnroe et al., Nature Nanotech. 2, 631 (2007)

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Project
05_EMINS_FP07_EuroSLAB / The rheology of the subducting slab and mantle (euroSLAB)

Mineral Physics and Chemistry of the Earth

A new description of the 3D dislocation core structure of forsterite by coupling Peierls-Nabarro and element-free Galerkin methods.

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The determination of the plastic properties of minerals is a key step to understand the workings of mantle convection. Plasticity is governed by the motion of dislocations, which is controlled by the spreading of the dislocation core. Many methods exist to model the dislocation core structure as the full relaxation of the atomic positions in a faulted crystal. Another way is the use of the Peierls-Nabarro (PN) model.

In this work we model the dislocation cores of forsterite, the magnesian end-member of (Mg,Fe)2SiO4 olivine, at the atomic scale using the Peierls-Nabarro model combined with a finite elements method (here, the element-free Galerkin method). This model is based on equilibrium between the elastic field of the dislocation and the inelastic forces acting on the glide plane of the defect. These inelastic forces derive from a misfit energy that can be calculated at the atomic scale by using the Generalized Stacking Faults (GSF) energy concept. The values of the GSF energy are obtained by shearing half of an infinite crystal over the other half. In this way, we obtain a model of the dislocation core profile and the value of the stress required to move a dislocation at 0K (the so-called Peierls stress).

Many experimental and numerical studies of the plasticity of forsterite have been performed. These studies show that deformation is dominated by the movement of [100] and [001] dislocations. In this study, we show that the [100] may exhibit non collinear dissociation in the (010) plane following the reaction reaction [100]-> 1/6[3 0 1] +1/6[3 0 -1]. We also discuss several possible core structures for [001] screw dislocations, including non-planar core spreadings and their response to stress.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

Topic: not applicable

Biomineralizationprozesses in foraminifera

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The possible cell physiological processes e.g. transport of ions to the site of calcification and distribution of organic membranes serving as templates for crystal nucleation will be discussed. An experimental approach investigating these processes in more detail will be presented.

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Topic: Atomistic Understanding of Minerals

Influence of pressure and coordination environment on bonding in bismuth sulphides: An ab initio study on Bi2S3 and Cu4Bi5S10

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A series of high pressure x-ray diffraction experiments have in recent years given us a detailed

knowledge about the crystal structures of sulfosalts and their evolution as a function of pressure [1].

The studied compounds contain Pb2+, Bi3+ and Sb3+ which have highly anisotropic coordination

environments due to their filled s-orbital in the valence shell.

With ab initio DFT calculations it is possible to model the electronic configuration of compounds

and study cation-anion interactions in detail [2] . We here present calculations on Bi2S3 at pressures

between 0 and 10 GPa. Focus is put on the anisotropy of the cation coordination environments.

Calculations on Cu4Bi5S10 are also presented in order to understand Bi-S interactions in different

coordination environments. Calculations are carried out with the Siesta ab initio code [3] and charge

density maps, PDOS, and COHP are used in the analysis of the results.

[1] L.F. Lundegaard, E. Makovicky, T. Boffa-Ballaran, T. Balic-Zunic, Phys. Chem. Min. 32 (2005)

578.

[2] A. Walsh, G. W. Watson, J. Solid State Chem. 178 (2005) 1422

[3] J.M. Soler, E. Artacho, J. Gale, A. García, J. Junquera, P. Ordejón, J. Phys. Condens. Matter 14

(2002) 2745.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

not applicable

Crystallography of calcite crystals in pearls

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A detailed study of a series of Polynesian pearls has revealed the presence of aragonite and calcite crystals in the basal pearl layer (Cuif et al., 2008). This finding challenges the classical scheme of mineralization in pearls with a continuous nacre production from the core to the outermost layer. Thus, the characterization of the crystalline structure of calcite and aragonite crystals is essential to understand mineralization of the basal layer in pearls. We have used a combination of scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) to analyze the crystallographic characteristics of calcite crystals. Preliminary results show that the calcite can be present in different forms (i.e. prisms) and crystallographic characteristics vary along with structural changes. An analysis of the crystallography data of calcite crystals will be provided and discussed with respect to pearl mineralization.

References:

J.P. Cuif, A.D. Ball, Y. Dauphin, B. Farre, J. Nouet, A.Perez-Huerta, M. Salomé and C.T. Williams. 2008. Structural, mineralogical, and biochemical diversity in the lower part of the pearl layer of cultivated seawater pearls from Polynesia. Microscopy & Microanalysis 14, 405-417.

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Project
05_EMINS_FP18_MINSUBSTRDYN /
Subgrain structure development in
rocks and metals (MINSUBSTRDYN)

Microstructure and Mineral Behaviour

Substructure dynamics in minerals and metals: New insights from experiments and numerical simulations

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The 2 year research effort of the EuroMinScI CRP “Substructure Dynamics in minerals and metals” has resulted in significant advancements in the knowledge and understanding of microstructural processes at the subgrain to grain scale. These advancements could only be achieved by development and implementation of innovative and unique experimental and numerical tools and iterative comparison of results from numerical models with “equivalent” physical experiments to improve our understanding of the processes under investigation. In the following, achievements within the project are summarized:

I) Knowledge and Understanding of substructure dynamics

A) In-situ annealing of substructure rich minerals show temperature dependent behaviour where boundaries of different morphology and orientation exhibit distinctly different characteristics.

B) Development of new concepts and models for a wide range of interactions of fluid inclusions with sub- and grain boundaries. Observations show that the range and complexity of interaction is much wider than previously thought.

C) Subgrain size and recrystallized grain size has a more complicated dependence on stress and temperature than expected and previously assumed; therefore, new models are required that take into account specific mechanisms of deformation, recovery and recrystallization in plastically anisotropic materials.

D) Subgrain misorientations can be used successfully in carefully controlled experimental sample suites to estimate the strain accommodated by dislocation creep. Thus these strain indicators are useful as gauges for the calibration of experimental flow laws for multi-mechanism creep.

F) We can now – a worldwide first - completely describe substructure characteristics in Ice

G) Documentation of substructure development in three dimensions during annealing

H) In depth understanding of ice deformation and recrystallization allowing predictions of ice behaviour at a wide range of natural conditions.

II) Innovative/ Unique Tool Development

A) Development of new transmitted light deformation cell with controlled fluid pressure system and internal load cell; high-resolution optical image analysis to quantify displacement fields in these experiments; real-time high resolution observations of substructure development in minerals and rock analogues

B) In-situ deformation, heating and cooling (for ice) experiments within an SEM with simultaneous EBSD analysis

C) In-situ annealing of salt single crystals using the 3DXRD analysis technique implemented at the Synchrotron Facility in Grenoble, France

D) Successful coupling between the N-Site FFT code and the ELLE modelling platform opening the opportunity to link subgrain and grain scale processes in anisotropic minerals and metals (e.g. new grain boundary migration (GBM) process driven by gradient of stored strain energy)

E) 3D numerical modelling system that can at present model anisotropic grain growth and will in the future incorporate processes now possible to model in 2D (see for example point C) above).

F) Development of numerical system to model changes in crystallographic orientation and subgrain boundary movement within individual grains.

III) Direct comparison of experimental and numerical results

A) Successful modelling of ice deformation experiments with numerical modelling using tool IID (see above) allowing prediction of ice deformation at a range of natural conditions

B) Iterative comparison and improvement of the numerical simulation code for nucleation and grain boundary migration using tool IID (see above)

C) Iterative comparison and improvement of the numerical simulation code for subgrain structure development using tool IIF (see above)

Present and future:

The CRP has achieved major advances in physics-based experimental techniques as well as pushed the boundaries of computer simulation on the subgrain and grain scale markedly further. Using these advances allows us to draw together the experimental and computational activities within the CRP into integrated, collaborative, innovative and novel research projects which significantly enhance our understanding of substructure dynamics and its interaction with grain boundaries. The directly comparison of results from physical experiments and numerical modelling and iterative improvement of the numerical code enables us to consolidate and verify our understanding of the physical laws governing sub- and grain scale processes and consequently predict material behaviour from microstructural development to rheological properties - beyond experimental - to natural conditions.

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Microstructure and Mineral Behaviour

First-principles simulation of spectroscopy in minerals under pressure.

Keith Refson
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Optical spectroscopy is one of the most important probes of mineral properties, particularly in the environment of a high-pressure cell. First-principles modelling using state-of-the-art ab-initio methods is an almost ideal partner to spectroscopic experiments, and when combined can offer considerable advantages. In particular a full assignment of infra-red, raman, or INS experiments is usually possible. I will present calculations illustrating the application of ab-initio spectroscopy to a variety of Carbonates, Silicates, Hydrides and Oxides.

Recent developments in the modelling of excited electronic states, notably Optimised Effective Potential methods show promise in addressing the limitations of local density-functional approximations for predicting band-gaps. I will present results on transition-metal oxide systems using OEP method, which compares favourably with hybrid exchange DFT for the prediction of optical bandgaps.

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Project
05_EMINS_FP08_MCEC / Mineralogy and Chemistry of Earth's core (MCEC)

Elements and Alloys at Extreme Conditions

Theory of alloys under high pressure and temperature: a supercell technique

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Importance of a proper description of alloys related to the Earth's core will be addressed and the supercell technique will be presented.

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Project
05_EMINS_FP18_MINSUBSTRDYN /
Subgrain structure development in rocks and metals (MINSUBSTRDYN)

Microstructure and Mineral Behaviour

On the Kinetics of Fluid Inclusions in Recrystallizing Rocks

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Fluid inclusions in minreal grains or grain boundaries provide fundamental information to help reconstruction of the conditions of basin formation and metamorphism (MCLIMANS 1987). The mobility of fluid inclusions and fluid-rock interaction helps us to characterize the effect of the pore fluid on i) the mechanical properties of the rock and ii) the transport of fluid through a rock volume.

It is often assumed that a rock volume that contains a fluid phase is considerably weaker than a dry rock volume (e.g. URAI 1983, SPIERS ET AL. 1990, KOHLSTEDT ET AL. 2003, SCHENK & URAI 2004, SCHENK ET AL. 2005, POST & TULLIS 1998). This weakening process is either chemically induced by enhanced diffusion processes and/or mechanically induced, as high pore fluid pressure leads to a reduction of the maximum strength of the overall rock volume (KRONENBERG & TULLIS 1984). Fluid movement is coupled with mass and energy transport resulting from fluid-rock interaction.

We study the kinetics of fluid inclusions using real-time observation in a transmitted light deformation apparatus with controlled pore pressure. Sample materials are rock salt (NaCl) and camphor ($C_{10}H_{16}O$) polycrystals, with a range of different fluids. Results show a number of possible interactions of fluids with grain and subgrain boundaries, deformation of fluid inclusions and large changes in grain boundary velocity during deformation and show many similarities with high-temperature, fluid-rich tectonites.

In the present study we focus on the effect of pore fluids with a high wetting angle with respect to the solid phase. In such a system we observe three partly coupled processes: i) the pore drag or Zener pinning, where a migrating grain boundary remains on a fluid-filled pore to lower the free energy, ii) pore drag, by which the pore remains attached to the moving boundary and iii) pore drop, where the pore is (partly) separated from the boundary and is left behind in the bulk crystal (PETRISHCHEVA & RENNER 2005).

Systematic measurements of grain boundary migration rates, evolution of crystal orientations and displacement fields in a series of experiments, in combination with analyses of the morphology of the grain boundary fluid and isolated inclusions provide an observational base for the numerical model ELLE. We developed a numerical code that provides us with information on the recrystallized texture in a polycrystalline material with respect to the pore fluid fraction and the mobility of isolated fluid inclusions.

Literature

HIRTH, G. & KOHLSTEDT, D.L. (2003): Rheology of the upper mantle and the mantle wedge: a view from the experimentalists. In: EILER, J.M (eds.): Inside the Subduction Factory, AGU Geophysical Monograph 138.

KRONENBERG, A. K. AND TULLIS, J. (1984): Flow strengths of quartz aggregates: grain size and pressure effects due to hydrolytic weakening. Jour. Geophys. Res. 89, 4298-4312.

MCLIMANS, R. (1987): The application of fluid inclusions to migration of oil and diagenesis in petroleum reservoirs. Applied Geochemistry, Vol. 2, 585-603.

PETRISHCHEVA, E. & RENNER, J. (2005) : Two-dimensional analysis of pore drag and drop.

Acta Materialia, 53, 2793-2803.

POST, A. & TULLIS, J. (1993): The rate of water penetration in experimentally deformed quartzite: implications for hydrolytic weakening

Tectonophysics 295, 117-137.

SCHENK, O. & URAI, J.L. (2004): Microstructural evolution and grain boundary structure during static recrystallization in synthetic polycrystals of Sodium Chloride containing saturated brine. Contributions to Mineralogy and Petrology 146, 671-682.

SCHENK, O. & URAI , J.L. (2005): The migration of fluid-filled grain boundaries in recrystallizing synthetic bischofite: first results of in-situ high-pressure high-temperature deformation experiments in transmitted light. Journal of Metamorphic Geology 23, 695-709.

SPIERS, C.J. & SCHUTJENS, P. (1990): Densification of crystalline aggregates by fluid-phase diffusional creep. - In: BARBER. D.J., MEREDITH, P.D (eds.): Deformation processes in minerals, ceramics and rocks. Unwin Hyman, 334-353.

URAI, J.L. (1983): Water assisted dynamic recrystallization and weakening in polycrystalline bischofite. Tectonophysics, Vol. 96, 125-157.

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Defects and Disorder in Minerals

On the existence of satellite reflections in natural nephelines

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As part of our research on natural nephelines nine samples of igneous origin from Scandinavia with chemical composition determined by EMPA were investigated by X-ray single crystal diffraction. The main goal of our experiments was to find samples showing satellite reflections the occurrence of which was described for the first time a half of century ago by Sahama [1].

The crystal structure of nepheline was solved by Hahn & Buerger in 1955 [2]. It is a stuffed derivative of tridymite. The idealized chemical composition of nepheline is KNa3Al4Si4O16 (space group P63). The alumosilicate framework consists of tetrahedral layers parallel to (001) containing six-membered rings. In more detail, two types of rings can be distinguished. One quarter of the rings (centred at 0 0 z) are quite regular (ditrigonal), whereas three quarters of the rings (centred at 0 ½ z) are strongly distorted (oval). The sequence of directedness of the tetrahedra in the single ring is UDUDUD. Within the nepheline structure, there are two different cation sites: potassium (coordinated by 9 oxygen atoms) is exclusively located in channels formed by the ditrigonal rings. On the other hand, the sodium cations preferentially occupy the oval channels and are coordinated by eight oxygen atoms.

The structure of our samples basically corresponds to that determined in [2]. They show a slight excess of Si, and some of them are rich in Fe (replacing Al in the structure). Si excess results in partially occupied K sites. T-O interatomic distances are indicating an ordered distribution of Al and Si. The refined occupancy parameters show a good agreement with the determined chemical composition. In difference to a previous study on the crystal chemistry of nephelines [3] all of our investigated samples are characterized by the presence of at least the strongest group of satellite reflections with indices ± ⅓; ± ⅓; ± 5.79. These reflections are more or less diffuse.

[1] Sahama, T. G. (1958) A complex form of natural nepheline from Iivaara, Finland. American Mineralogist, 43, 165-166.

[2] Hahn, T. & Buerger, M. J. (1955) The detailed structure of nepheline, KNa3Al4Si4O16. Zeitschrift für Kristallographie, 132, 45-70.

[3] Tait, T. K., Sokolova, E., Hawthorne, F. C., & Khomyakov A.P. (2003) The crystal chemistry of nepheline. Canadian Mineralogist, 41, 61-70.

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Microstructure and Mineral Behaviour

The HydroMin-project

Bjoern Winkler

The aim of the HydroMin project is to increase our understanding of structure-property relations of hydrous and nominally anhydrous minerals and of the incorporation of hydrogen into nominally anhydrous minerals by modelling and experiment. The studies we have performed include the synthesis of nominally anhydrous compounds, the experimental determination of diffusion coefficients and inelastic x-ray spectroscopic experiments. Modelling studies included investigations of the lattice dynamics, including the effect of anharmonicity and the study of absorption coefficients. I will give an overview of the progress made in the last two years within the CRP.

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Microstructure and Mineral Behaviour

Defects and deformation in olivine: from molecules to mantle

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The rheological properties of olivine, the most abundant mineral in the Earth's upper mantle, are profoundly influenced by the presence of water. We are currently using a multi-scale approach that combines experiment and theory to determine the manner and degree to which water influences the properties of olivine. Our methodology embraces plate-scale modelling of lithospheric deformation with characterisation of microstructures in deformed mantle rocks and atomic scale modelling of water related defects in olivine. An overview of the project will be given, along with new results.

CONFERENCE ABSTRACTS - POSTERS

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Topic: Atomistic Understanding of Minerals

Description of modular minerals within the superspace approach

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Modular structures are frequently observed in the mineral world. These structures are built of modules, approximately described by simpler structures. The Pb-Bi-Ag sulphosalts of the lillianite homologous series are examples of modular minerals based on PbS-like structure. The fact that the structure of these minerals can be described with the help of a simple average structure in combination with additional small distortions moved us to explore the potential of the so-called superspace approach for their description. The superspace formalism was originally developed for the study of modulated structures and is by now a well established tool for the treatment of incommensurately modulated structures, composite crystals or quasicrystals. But superspace is also a powerful and efficient tool for dealing with the structural properties of commensurate systems with large unit cells. A necessary condition is that the structures have approximate much smaller subperiodicities, which is the case for modular structures. The superspace formalism allows a unified description of whole homologous series, with the number of structural parameters smaller than in a conventional approach, and predicts the observed three dimensional space groups of individual members. With the introduction of some new concepts we have successfully applied the superspace method to the analysis and refinement of the lillianite homologues. The structures are best described as modulated structures, but with unusually large displacive modulations of a linear "zig-zag" type. An efficient treatment required the modification of the refinement program JANA2006 in order to introduce this type of functions as alternative basic modulations.

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Project
05_EMINS_FP18_MINSUBSTRDYN / Subgrain structure development in rocks and metals (MINSUBSTRDYN)

Topic: Microstructure and Mineral Behaviour

3D modelling of grain boundary migration

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Microstructures of rocks play an important role in determining rheological properties and help to reveal the processes that lead to their formation. Some of these processes change the microstructure significantly and may thus have the effect of obliterating any fabrics indicative of the previous history of the rocks. One of these processes is grain boundary migration (GBM). During static recrystallization, GBM may produce a foam texture that completely overprints a pre-existing grain boundary network and GBM actively influences the rheology of a rock, via its influence on grain size and lattice defect concentration.

We introduce here a new 3D simulation software that is capable of modeling a range of physical processes on the grain scale over time using a front-tracking model.

Front-tracking methods are a class of techniques that can be applied to simplify interface problems. Using the front-tracking approach, the problem can be solved analytically by linear equations by specifically tracking the evolution of boundary "fronts". The front-tracking approach is therefore ideally suited for the purpose of modelling GBM.

The underlying principle of this new 3D simulation software is the definition of grains as mathematically precise polyhedra. Each polyhedron is described by an independent set of vertices, edges and facets. This has the great advantage that polyhedra can be taken out of the structure for a more precise and faster analysis of its properties (e.g. angles between facets, area of facets, development of a single facet or a whole set of facets etc.) or evolution. Each topological characteristic (vertices, edges and facets) and the polyhedron itself can have an unlimited number of properties (such as surface energy, chemical potential, orientation, mineral type etc.).

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Project
05_EMINS_FP18_MINSUBSTRDYN /
Subgrain structure development in
rocks and metals (MINSUBSTRDYN)

Topic: Microstructure and Mineral Behaviour

Substructure dynamics during annealing: Complex temperature dependent behaviour revealed by in-situ heating experiments

Verity Borthwick, Sandra Piazolo, Gill Pennock, Colin Peach
VB and SP at Stockholm University, GP and CP at Utrecht University

Substructure dynamics during annealing: Complex temperature dependent behaviour revealed by in-situ heating experiments

Verity Borthwick, Sandra Piazolo, Gill Pennock and Colin Peach

Static in-situ annealing of a deformed single-crystal halite shows that three distinct temperature dependent stages of dislocation rearrangement result in an overall decrease in the crystallographic variation of the sample.

Substructure dynamics have been investigated in “real-time” by in-situ heating experiments conducted in the SEM. Electron Backscatter Diffraction (EBSD) maps were taken before, during and after each heating stage, to collect detailed information about the crystallographic orientation and misorientation of the sample substructure. Samples were pre-deformed under uniaxial compression at a temperature of ~450 ºC to strains of 0.165, at a strain rate of 6.9*10-6s-1. Samples were then annealed within an SEM in several heating stages at temperatures between 280-470 ºC, with an arbitrary increase in temperature at each heating stage. The length of each heating stage varied from 30 minutes to six hours.

Behaviour during annealing of halite can be divided into three distinct phases based on the low-angle boundary (LAB <15º) behaviour and overall changes in the substructure. LABs were divided into five categories based on their morphology, orientation and behaviour. Characteristic behaviour of the annealing phases are:

Annealing phase one at <300 ºC

(a) increase in the misorientation of LABs aligned with (011) and (0-11) slip planes

(b) decrease in the misorientation of LABs aligned with (-101) and (101) slip planes and

short, detached LAB segments

(c) boundary movement as much as 7µms by a small number of LABs

(d) subdivision of some subgrains into plateaus of like orientation

Annealing phase two ~300 ºC

(a) continuing increase of (011) and (0-11) aligned LABs

(b) larger decrease by other LAB types with some detached segments dissipating

(c) significant decrease in boundary movement to <1µm

(d) continued subdivision of subgrains and formation of new LABs at plateau borders

Annealing phase three >300 ºC

(a) increase in misorientation of all remaining LABs

(b) largest amount of boundary movement, as much as 12.5µms

(c) no new plateau formation occurs

We suggest that annealing behaviour is both temperature dependent and varies according to which boundary is examined. At lower temperatures (T<300 ºC) annihilation of dislocations in the subgrain interior and at the boundary site for LABs aligned with the harder slip system occurs, resulting in a decrease in misorientation. Concurrently, dislocations are added into the boundaries in the preferred alignment, which then increase in misorientation. In areas where there are no dislocations of opposite sign, annihilation is not possible and dislocations of like sign begin to align. Consequently, next to these aligned dislocations plateaus of like orientation form. Phase two (T~300 ºC) marks the peak of behaviour exhibited in phase one, as temperature increase extends the length scale on which dislocations are attracted to boundaries. New tilt boundaries form at borders of plateau regions as more dislocations are added. At T>300 ºC changes are dominated by LAB development, where remaining dislocations move towards boundaries as the range of attraction increases further. The cumulation of these processes results in an overall decrease in the crystallographic variation of the sample and thus a significant decrease in the stored energy of the system.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

Topic: not applicable

Organic matrices of carbonate skeletons: biochemical analyses of extracted matrices and in situ characterization at a micron scale level

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The main mineral components of CaCO3 Mollusc shells and coral skeletons are calcite and aragonite. It is well-known they are associated with organic components, the diversity of which reflects the taxonomic diversity.

Mollusc shells are composed of several layers, the mineralogy, number and arrangement of which are species dependant. These structures have been classified (Boggild, 1930): prismatic, nacreous, crossed lamellar layers, etc. SEM and TEM observations have shown the units (prisms, tablets, fibres or laths) are composites. Coral skeletons (Scleractinia) are composed of aragonite early mineralizing zones (EMZ) and fibres. Growth layers 1-3 μm thick are present in all these skeletons.

Organic components are present as envelopes surrounding the microstructural units (intercrystalline organic matrices, IOM), and within the units (intracrystalline, soluble organic matrices). Biochemical analyses of the extracted organic matrices have shown that the main components are proteins and sugars, depending upon the taxa. Intercrystalline membranes are layered, and show a growth zonation. Soluble organic matrices (SOM) extracted from corals are mainly composed of acidic sulphated sugars (similar to chondroitin sulphate), whereas proteins are the main components of aragonite nacreous and crossed lamellar layers of Molluscs. The SOM of the large calcite prisms of Pinna and Pinctada clearly differ despite their overall similarities: highly acidic sulphated sugars in Pinna, proteins in Pinctada. In contrast to the intensive study of proteins as components of the mineralizing matrices involved in crystallization, sugars received relatively few attention. Usually said to be negligible, lipids are detected using specific extraction processes. As for proteins and sugars, they seem dependant upon the species.

In situ analyses at a micron scale are now available. WDS, EDS and NanoSIMS maps show that microstructural growth layers correspond to chemical zonations. Infrared maps display the complex compositions of each layer and intercrystalline organic membranes. Thick intercrystalline membranes are chemically layered, and show discontinuities related to the growth zonation. XANES maps at the S K edge of coral and mollusk skeletons confirm the presence of organic sulphate, and S amino acids, as well as their chemical zonation. TOF SIMS maps also display intracrystalline heterogeneities as well as the complex structures of the intercrystalline organic envelopes.

Oscillations of compositions (Mg, Sr, sulphated polysaccharides...) are linked to the daily rhythm of crystallization in the shells of Mollusks and coral skeletons, both taxa used as proxies for palaeoenvironmental reconstructions. AFM images show that all these layers are composed of rounded granules with a cortex, or envelope, about 8 nm thick. From what is known of the organo-mineral composition of shells, it may be suggested that this cortex is composed of organic matrix and/or amorphous calcium carbonate, and that the organo-mineral granules are heterogeneous. Although prisms, nacreous tablets, laths... are seen as monocrystals, they are composite. This implies that an improved understanding of the calcareous biocrystallization process requires investigations at the submicrometric scale of the growth layer.

Guzman N., Ball A.D., Cuif J.P., Dauphin Y., Denis A., Ortlieb L., 2007 - Microsc. Microanal. 13: 397-403.

Dauphin Y., Ball A.D., Cotte M., Cuif J.P., Meibom A., Salomé M., Susini J., Williams C.T., 2008 - Anal. Bioanal. Chem. 309: 1659-116.

Dauphin Y., Cuif J.P., Williams C.T., 2008 - Comp. Biochem. Physiol. B150: 10-22.

Cuif J.P., Ball A.D., Dauphin Y., Farre B., Nouet J., Perez-Huerta A., Salomé M., Williams C.T., 2008 - Microsc. Microanal. 14: 405-417.

Farre B., Dauphin Y., in press - Lipids from the nacreous and prismatic layers of two Pteriomorpha Mollusc shells. Comp. Biochem. Physiol.

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Project
05_EMINS_FP13_MICROMAGN /
Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

Topic: Microstructure and Mineral Behaviour

Clusters and holes: Exchange networks in hematite-ilmenite solid solutions

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Holes and clusters of exchange networks dominate the low-temperature, metastable phase diagram of the system (1 – X) Fe_2O_3-X $FeTiO_3$ (IlmX). By our measurements we have probed and extended the phase diagram of Ishikawa et al. (1985) in the light of magnetic influences of the random exchange links, which originate either by replacing random pairs of Fe^{2+} and Ti^{4+} ions in the ordered ilmenite lattice by two Fe^{3+} ions (ordered IlmX phase), or by randomly replacing two Fe^{3+} ions in the hematite lattice by a pair of Fe^{2+} and Ti^{4+} ions (disordered IlmX phase). Now a large dataset is available from these measurements, and we propose several new ideas to interpret the sometimes unexpected results. By refining a method of Ishikawa (1967), we analyze the PM' region of the phase diagram in terms of a mean field theory of interacting clusters. This allows to determine cluster sizes and interaction field distribution by inverting hysteresis measurements of Ilm 92 and Ilm97. To understand the relation between ordered and disordered phases we use a mean field theory to determine Neel and Curie temperatures of both. An especially interesting finding is that the experimentally observed intersection of PM-PM' crossover with the AF phase boundary close to Ilm97 can be explained by analyzing average exchange interaction strengths.

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Project
05_EMINS_FP05_BIOCALC /
Calcareous Biocrystals (BioCalc)

Topic: not applicable

Insights of the specificities of the nacre-prism transition in the pearl oyster Pinctada margaritifera

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Proteins S Sugars S

The Mollusc shell is commonly described as a two layered structure: an outer layer composed of calcite prisms and an internal aragonitic nacreous layer. This long standing oversimplification is due to the remarkable appearance of the few species in which this simple structural arrangement is illustrated. The Pelecypods belonging to the genus Pinctada, the "pearl oysters" are the best known. The calcite prisms of the external layer are easily visible as units perpendicular to the shell surface. This organisation of the external layer is in clear contrast to the finely layered aragonite with tablets parallel to the shell surface.

Previous data have shown clearly different biochemical compositions. Not only proteins and sugars are present, but lipids are also detected and seem dependant upon both structure and species (Farre & Dauphin in press).

Early observations by Wada (1957) had suggested that a transitional material may exist between the prismatic and nacreous layers of Pinctada martensi.

A multi-analytical study shows that the nacreous-prismatic boundary in the shells of Pinctada margaritifera is not abrupt. The mineralogy and chemical compositions of this zone are indicative of a fibrous aragonitic layer with growth lines. Results from confocal microscopy, EPMA, XANES and infrared maps show that the organic components of this layer are similar to those of the nacreous layer. However, the changes in the biomineralization process are not restricted to this fibrous aragonite layer. Infrared, XANES and NanoSIMS and some element maps also show that the composition of the final growth stage of the prismatic layer is different from the main part of this layer. These results are confirmed by TOF-SIMS maps. Several organic components are only highlighting the microstructures, but some others also show that the transition between prisms and nacre is a complex process. The end of the prismatic layer and the beginning of the nacre both display singularities in their chemical compositions, regarding mineral compounds as well as organics. We have identified at least three stages of growth from the prismatic structure to the nacreous layer. First, a change can be seen in the chemical and biochemical composition of the last growth increments of the prisms, although no change is visible in the microstructure or in the mineralogy. Secondly, there is a change in the mineralogy and structure, and the chemical composition becomes similar to that of the nacreous layer, except some specific compounds revealed by TOF-SIMS. Finally, the microstructure becomes the nacreous layer, with the formation of the regular tablets. There is a good correspondence between the histological areas identified by Jabbour-Zahad et al. (1992) and the three step biomineralization process outlined here.

Wada K (1957) Bull Natl Pearl Res Lab 2: 86-93.

Jabbour-Zahab R., Chagot D., Blanc F., Grizel H. (1992) Aquat. Living Res. 5: 287-298.

Farre B., Dauphin Y. (In press) Comp. Biochem. Physiol.

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Project
05_EMINS_FP11_ORION / Ordering of Ions in Minerals (ORION)

Topic: Defects and Disorder in Minerals

X-Ray powder diffraction of synthetic Al-rich phlogopites: lattice parameters, polytypes, stacking faults, and implication of modulations

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X-ray powder diffraction experiments of synthetic Al-rich phlogopites synthesized at 800 °C and 2 kbar were carried out. The grain size of the synthetic phlogopites ranges between particle diameters of 3 to 5 µm. The samples have already been well characterized by solid state NMR spectroscopy, and thus, possible impurity phases have been assigned.

As for all micas, the phlogopite structure can be described in terms of the OD-theory, where 2-d periodic layers can be stacked in different ways without changing the transition from one layer to the adjacent one (Nespolo and Ďurovič 2002).

One aim of the experiments was to study the change of lattice parameters with increasing F- and Al-content. Previous investigations have already shown that the c-lattice parameter decreases strongly with increasing F-content (e.g., Papin et al. 1997). From combined powder XRD and TEM investigations we expect to get detailed information on the polytypes which were formed during synthesis and on stacking faults in the mica structure. Up to now, many natural phlogopite single-crystals and synthetic powder samples have been characterized using XRD techniques. The most common polytype is the one-layer monoclinic polytype (1M) with space group symmetry C2/m. The other two possible polytypes, 2M1 (space group symmetry C2/c) and 3T (space group symmetry P3112) are far less abundant (Brigatti and Guggenheim 2002).

Our first refinements indicate that all phlogopite samples consist of polytype 2M1. However, there may also be a mixture of polytype 2M1 and polytype 1M, leading to inelastic X-ray scattering. In some powder patterns with better resolution, satellite reflections surrounding hkl-reflections occur, which have not yet been reported and imply the presence of a modulated structure.

We expect that the X-ray diffraction results will be a valuable complement to our solid-state NMR investigations. While solid-state NMR spectroscopic investigations offer an insight into the local structure of the nuclei, the powder XRD patterns refinements may give new information about the long-range order of the tetrahedral and octahedral sheets. Combined with the TEM investigations, the results will contribute to a better understanding of stacking faults in the mica structure. Furthermore, this information may clarify the presence and type of modulations in the structure.

References

Brigatti, MF, Guggenheim, S (2002) In: Reviews in Mineralogy and Geochemistry 46: 1-90

Nespolo, M, Ďurovič, S (2002) In: Reviews in Mineralogy and Geochemistry 46: 155-272

Papin, A, Sergent, J, Robert, JL (1997) Eur. J. Min. 9: 501-508

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Project
05_EMINS_FP21_HYDROMIN / Hydrogen in Minerals (HydroMin)

Topic: not applicable

Water solubility in diopside

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Diopside is one of the end members of omphacite. Omphacite from mantle xenoliths shows the highest concentration of hydroxyl in its structure among other nominally anhydrous minerals. Moreover, omphacitic clinopyroxenes may transport water deeper into the mantle after the breakdown of hydrous minerals in subducted slabs. Water solubility in orthopyroxene is known to strongly increase with Al content. Therefore, aluminous clinopyroxenes may actually play an important role in recycling water back into the mantle. In this study, we looked at water solubility in both pure diopside and in diopside containing variable proportions of aluminum.

For all experiments with pure diopside, water contents were relatively small, in the order of several hundreds ppm of water. All measured infrared spectra of pure diopside fall into two groups. The first group of bands (Type I) occurs at higher wavenumber, at 3650 cm-1, the second group (Type II) at lower wavenumber, at 3480-3280 cm–1. The appearance of Type I or Type II spectra was neither correlated with pressure or temperature. The differences in the spectra point towards substitution mechanisms involving different vacancies, which in turn could be the result of different oxide activities in the starting material. Therefore, a separate series of experiments was carried out with starting materials with an excess or deficiency of MgO or SiO_2. These experiments yielded diopside with different absorption spectra. Starting materials with low silica activity yielded Type I bands, which are therefore likely to be related to Si vacancies. Type II bands form at high silica activity and may therefore be related to Mg or Ca vacancies. All spectra of both types show the same polarization behavior with the highest absorption in β direction, almost identical but slightly smaller absorption parallel to γ, and the lowest absorption along the α axis of the indicatrix.

All infrared spectra of the Al-containing diopside show one main absorption band at 3650 cm-1. It means that only one type of substitution mechanism takes place. The water solubility strongly increases with the presence of Al up to 2500 ppm H_2O. The results on temperature dependence of water solubility in Al-bearing diopside show that water solubility decreases with increasing temperature. Estimated partition coefficients of water between clinopyroxene and orthopyroxene are close to unity, with Dcpx/opx possibly increasing with temperature.

Due to the low solubility of aluminum in clinopyroxene at high pressure, the data on pure diopside are probably a good guide for the water solubility in clinopyroxenes under the conditions of the deeper upper mantle. Since water solubility in diopside under those conditions is order of magnitude below the water solubility in olivine, clinopyroxene is not expected to be a major storage site for water in the deeper upper mantle, even if its modal abundance is significant.

Together with previously published data on water in orthopyroxene, the results of this study clearly show that in the uppermost mantle, most of the water is dissolved in the pyroxenes. The relative importance of clinopyroxene and orthopyroxene is primarily a function of their modal abundance. This observation is consistent with the model of Mierdel et al (2007) [1], which suggests that the Earth's asthenosphere is due to a minimum in water solubility in nominally anhydrous minerals.

[1] Mierdel K., Keppler H., Smyth J., Langenhorst F. (2007) Water solubility in aluminous orthopyroxene and the origin of Earth's asthenosphere. Science. 315. 364-368.

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Project
05_EMINS_FP13_MICROMAGN /
Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

Topic: Microstructure and Mineral Behaviour

Understanding crustal magnetic anomalies by mapping magnetic interactions from nanometer to millimeter scale

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Magnetic exploration on local and global scale is focused on interpreting magnetic anomalies in terms of induced magnetization in today's geomagnetic field. However, numerous anomalies in Norway, Sweden and USA originate from rocks with oxide exsolution intergrowths with a magnetic response, which is dominated by a magnetic remanence acquired many million years ago.

Different minerals control induced versus remanent magnetization. Little is known about the detailed interplay between them. Using the newly developed technology of a giant-magnetoresistance micro-scanner it is now possible to map remanent and induced magnetization at the mineral size-scale from 10 micron up to several millimeters. At the start of the MICROMAGN project we had proposed a new type of magnetization, Lamellar Magnetization (LM), to account for magnetization of these unusual rocks. Based on the results from magnetic measurements and modeling, Monte Carlo simulations, DFT calculations made in the course of the project LM is now a robust theory. Now our goal is to understand how the interface moment (LM) changes with temperature and pressure in crustal rocks and how magnetic anomalies will be effected by these changing conditions.

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Project
05_EMINS_FP21_HYDROMIN /
Hydrogen in Minerals (HydroMin)

Topic: Atomistic Understanding of Minerals

Anharmonic OH vibrational frequencies in simple hydroxides

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The physical properties of hydrous minerals are found strongly dependent on the hydrogen interaction and the nature of the OH group in the crystal. Many of the central research problems in such inorganic materials therefore involve the identification of OH defects and the characterization of the local structure and bonding around the OH groups. Here vibrational spectroscopy (IR and Raman) is one of the major research tools. The present contribution uses "computational vibrational spectroscopy".

LiOH and Mg(OH)2 are two examples of the (abundant) class of hydroxides which contain layers of OH groups which “bond” towards each other in an anti-parallel fashion across the inter-layer gaps. Both crystals display interesting vibrational features, which will be discussed in this poster, based on results from theoretical calculations.

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Project
05_EMINS_FP13_MICROMAGN /
Magnetism and microstructure: from the nanometre to the planetary scale (MICROMAGN)

Topic: Microstructure and Mineral Behaviour

Effect of strain and magnetic interaction parameters in the hematite-ilmenite system

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Density functional theory calculations including a Hubbard U give first theoretical evidence for the lamellar magnetism hypothesis [1]: The polar discontinuity at the interface in Fe2O3/FeTiO3 heterostructures is accommodated through Ti4+ and a disproportionation in the Fe contact layer into Fe2+, Fe3+[2].

By straining Fe2O3/FeTiO3 heterostructures and solid solutions to the lateral constant of different substrates (e.g. Fe2O3(0001), FeTiO3(0001), Al2O3(0001), Ag(111)) and relaxing the c/a ratio, we explore the effect of strain and find that is has a profound influence on the electronic properties: While at aFe2O3 the impurity levels are pinned at the Fermi level leading to halfmetallic behaviour [2], at aAl2O3 they shift to lower energies and the system remains insulating. This opens a path to tune the properties of the heterostructure by varying the substrate material.

Furthermore, magnetic exchange interaction parameters of the end members are extracted by mapping the DFT total-energy difference of various spin-configurations on a Heisenberg Hamiltonian. These parameters will be used as input for kinetic Monte Carlo simulation to obtain a comprehensive understanding of magnetism on multiple scales.

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[1] P. Robinson, R.J. Harrison, S.A. McEnroe, and R. B. Hargraves, Nature 418, 517 (2002).

[2] R. Pentcheva, H. Sadat Nabi, “Interface magnetism in Fe2O3/FeTiO3-heterostructures”, Phys. Rev. B, 77, 172405 (2008)

[3] H. Sadat Nabi, R. Pentcheva, “Structure and electronic properties of Ilmenite: a GGA+U study” in preparation.

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