

EuroMinSci open session at the EGU General Assembly 2007

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GMPV20/BG5.10 – Mineral properties and behaviour: the European Mineral Sciences Initiative (EuroMinSci) open session (including the EMU Research Excellence Medal Lecture) (co-organized by BG) (co-listed in CR, NP, SSP)

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Session co-sponsored by the ESF-EuroMinSci Programme (www.esf.org/eurominisci)

Session Abstract

Major advances in the use of physics-based experimental techniques (nuclear magnetic resonance spectroscopy, synchrotron radiation, neutron scattering, phonon spectroscopy, laser-ablation based techniques, etc.) and atomistic computer simulation make it possible to study mineral properties and behaviour. In addition, measurements of many minerals properties in situ at extreme conditions of temperature and pressure corresponding to those existing in the earth's interior are now feasible (e.g., the recent, experimental and theoretical determination of the temperature at the inner core – outer core boundary and the study of the Earth's core chemistry). The EuroMinSci Programme draws together the experimental and computational activities, and the different experimental techniques, into integrated research projects in this field. It focuses on the atomistic understanding of structures, properties and processes of minerals. This open session will offer in particular an overview of the EuroMinSci programme, which is supported by national funding agencies from 10 European countries from Austria (FWF), Belgium (FWO, FNRS), Czech Republic (CSF), Estonia (ETF), France (CNRS), Germany (DFG), Hungary (MTA), Italy (CNR), Slovakia (SAV), Spain (MEC), Sweden (VR), United Kingdom (NERC), and the European Science Foundation (ESF), thanks to contract ERASCT-2003-980409 of the EC, DG Research.

Session Conveners

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Oral Programme

Tuesday, 17 April 2007; Lecture Room: Lecture Room 20 (N)

Chairperson: Bjoern Winkler

13:30 - 13:45 – Winkler, B.; Friedrich, A.; Wilson, D.; Haussühl, E.; Refson, K.; Probert, M.; Gale, J.; Milman, V.
Structure and properties of hydrous minerals from experiment and computation

13:45 - 14:00 – Calvet, M.; Margerin, L.
Calculation of effective seismic properties of untextured crystal aggregates and application to inner core crystallisation

14:00 - 14:15 – Fabian, K.; McEnroe, S.; Robinson, P.
Lamellar magnetism carries the natural remanent magnetization in ilmenohematite from Modum, Norway

14:15 - 14:30 – Kantor, I.; Dubrovinsky, L.; McCammon, C.

Pressure-induced spin crossover in ferropicase: an alternative concept.

14:30 - 14:45 – Friedrich, A.; Haussuehl, E.; Wilson, D.J.; Boehler, R.; Morgenroth, W.; Winkler, B.; Juarez-Arellano, E.A.; Refson, K.; Milman, V.

Structure and properties of diaspore, AlO(OH), up to 50 GPa from experiment and theory

14:45 - 15:00 – Walte, N.P.; Heidelbach, F.; Rubie, D.C.; Frost, D.J.

LPO and Perovskite–post-Perovskite phase transition of CaIrO₃ during deformation with the d-DIA: Implications for the D'' layer

Chairperson: Bernard Avril.

15:30 - 16:00 – Bindi, L.

From the invalidity of the law of rational indices to the concept of superspace: A crystallographic excursion in the modulated world of minerals; solicited - EMU Research Excellence Medal Lecture

16:00 - 16:15 – Olsen, LA; Balic-Zunic, T; Makovicky, E

From lillianite to α -Pb₃Bi₂S₆: a crystal chemical study of Pb₃Bi₂S₆ at high pressure

16:15 - 16:30 – Cuif, J.P.; Dauphin, Y.; Nouet, J.

Nano-crystallization within chemically active glyco-protein hydrogel layers: a possible origin for the long-standing vital effect enigma in the Ca-carbonate skeletons.

16:30 - 16:45 – Blanchard, M.; Wright, K.

Incorporation modes of hydrogen in ringwoodite: a DFT study

16:45 - 17:00 – Tatham, D.; Prior, D.

In situ heating and deformation experiments in the SEM

Poster Programme

Poster Area: Hall A

Display Time: Tuesday, 17 April 2007 08:00 - 19:30

Author in Attendance: Tuesday, 17 April 2007 08:30 - 10:00

A0105 – Avril, B.

EuroMinSci Programme - An overview

A0106 – Perchuk, A.; Schertl, H-P.; Burchard, M.; Maresch, W.V.; Gerya, T.V.; Bernhardt, H-J.

Diffusivities of major divalent Cations in Gem quality and chemically heterogeneous Garnets: multi-couple Experiments

A0107 – Perchuk, A.; Vidal, O.

Diffusion couple Experiments in Garnets: Effect of grain boundary Diffusion owing to 2D numerical Modeling

A0108 – Prokof'ev, V.; Baksheev, I.; Zorina, L.; Kryazhev, S.

Conditions of tourmalinization formations Eastern Transbaykalia gold deposits, related with mesozoic riftogenic volcanism (Russia)

A0109 – Fabian, K.; Shcherbakov, V. P.; McEnroe, S.; Robinson, P.

A mean field model of the magnetic structure in hematite-ilmenite solid solutions and exsolved nanostructures of ilmenite and hematite

A0110 – Méheut, M.; Lazzeri, M.; Balan, E.; Mauri, F.

Prediction of stable isotopes fractionation by first-principles methods

A0111 – Deguen, R.; Alboussière, T.; Brito, D.; La Rizza, P.; Masson, J.-P.

Ultrasonic monitoring of dendritic solidification under a pressure gradient

- A0112 – Becker, JKB; Bons, PDB
A new approach to 3D front-tracking simulation of grain growth
- A0113 – Pennock, G.M; Drury, M.R.
The effect of deformation on subgrain misorientations
- A0114 – Nouet, J.; Cuif, J.P.; Pradel, P.
Differential crystallization of high-magnesian calcites in the cortical spicules and axes of the red coral (Corallium rubrum) correlated to the biochemical compositions of their mineralizing matrices
- A0115 – Nehrke, G.; Van Cappellen, P.; Bijma, J.
Calcite growth rate and solution stoichiometry, implications for biomineralizations
- A0116 – Dauphin, Y.; Cusack, M.; Ortlieb, L.
Nanogranules in carbonate skeletons: a universal scheme?
- A0117 – Valcke, S.L.A; Drury, M.R.; Pennock, G.M.; De Bresser, J.H.P
Quantifying heterogeneous microstructures: core and mantle subgrains in deformed calcite
- A0118 – Griera, A.; Jessell, M. W.; Evans, L.
Simulation of subgrain scale deformation and its effect on recrystallisation
- A0119 – Brigatti, M.F.; Malferrari, D.; Poppi, M.; Mottana, A.; Cibin, G.; Marcelli, A.; Cinque, G.
Interlayer potassium and its surrounding in micas: Crystal chemical modeling and XANES spectroscopy
- A0120 – Dubacq, B.; Vidal, O.; Lewin, E.; Vieillard, P.
Prediction of enthalpy of formation of minerals: application to solid solutions and low-temperature compounds
- A0121 – Yuditsev, S.; Livshits, T.; Omelianenko, B.
Examination of natural and synthetic minerals as matrices for actinide waste immobilization
- A0122 – Sendir, H.; Saryiz, K.
Geochemistry and mineralogy of the chromitites and their platinum group minerals in the Karaburhan (Sivrihisar-Eskipehir-Turkey) region
- A0123 – Krivolutskaya, N.A.; Sobolev, A.V.; Kuzmin, D.V.; Svirskaya, N.M.
Olivines composition data to the origin of the Noril'sk deposits (Siberian trap province, Russia)
- A0124 – Zarrinkoub, Dr
Antimony – gold mineralisation and structural controls in south Nehbandan, East of Iran
- A0125 – Zareisahamieh, R
Mineralogical and Geochemical Characteristics of Tafresh(Central Iran)
- A0126 – Seaman, S.; Helfrich, E. ; Dyar, D.; Smith, R.
Synchrotron FTIR analysis of water concentration variations in skeletal sanidine crystals hosted by spherulites in the Hell's Gate rhyolitic lava flow, southern Arizona, USA
- A0127 – Hamann, I.; Azuma, N.; Weikusat, Ch.
Evolution of ice crystal microstructures during creep experiments
- A0128 – Salje, E.K.H
Fast Ionic Transport along Interfaces in Minerals
- A0129 – Hagh Nazar, M.; Esmaeily, E.; Kosari, A.
Electron microprobe and mineralogy evidence for the genesis of Scheelite and Tourmaline at the Nezamabad area, western Iran