

Scientific Report of the 'Networking activity' within the

ESF-EUROCORES EuroMinSci

'Co-sponsoring of sessions at the **Frontiers in Mineral Sciences 2007** meeting'

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1 Background /Justification for Application as a networking activity

The ESF EUROCORES 'European Mineral Science Initiative' provides a framework for integrating atomistic modeling and experimental studies in the field of Mineral Physics. The ESF, with funds from the EC Sixth Framework Programme under contract no. ERAS-CT-2003-980409, provides support for networking activities of funded projects. Eight international and one associated national collaborative research project, comprising about 80 principal investigators, are involved.

The 'Frontiers in Mineral Sciences 2007' meeting in Cambridge (UK) was conceived as an international meeting for the presentation of recent advances in science across the broad remit of mineralogy. It was, for the first time, a meeting organized jointly by the Mineralogical Society of Great Britain and Ireland, the Mineralogical Society of America, the Mineralogical Association of Canada and the Société Française de Minéralogie et de Cristallographie.

Obviously, the scope of the conference was a superset of the scientific aims of EuroMinSci. Also, several people involved in the organization of the Frontiers meeting, especially M. Carpenter and E. Artacho, have links to EuroMinSci. Hence, a co-sponsoring of sessions and a general support of the meeting was seen as an efficient way to present EuroMinSci to the international mineralogical community, to provide a framework in which members of different CRPs could come together and discuss their projects and where the science done in the framework of EuroMinSci could be placed in an international context. It was also seen as an opportunity to continue planning of joint EuroMinSci activities.

2 Application for ESF funding

The proposal to co-sponsor two sessions and contribute to local organization costs was put forward by B. Winkler (PL HydroMin), R. Harrison (PL MicroMagn) and M. Carpenter. An initial request for indication of interest in participation in the conference resulted in about 15 members of EuroMinSci stating their intent to participate. On this basis, 22.680 € were initially requested from the ESF, in order to be able to financially support the participation of 15 European members, 1 Australian associate and 2 external speakers (Prof. J. Gale, Curtin

University, Western Australia and Prof. J. Kirschvink, California Institute of Technology, California).

After the networking activity was approved by the SC, a final call for applications led to 27 EuroMinSci investigators to express their interest. The flexibility of the ESF to adapt the budget accordingly was very helpful, and a total of 35.000 € was approved. Of this, 2.200 € were directly transferred from the ESF to the organizers as a contribution towards local expenses.

3 The Frontiers 2007 meeting

3.1 General

At the meeting 257 oral and 125 poster presentations were presented in 19 thematic sessions at the Fitzwilliam College Conference Center. The meeting attracted about 400 participants from 26 different countries. A book of abstracts has been published, with a prominent advertisement of the ESF as a co-sponsor on the first page and an extended presentation of the ESF, EUROCORES and EuroMinSci on page 2.

3.2 Participation by members of EuroMinSci

In the end, 20 participating EuroMinSci members requested support:

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| MicroMagn | Harrison, Palin, Pentchava, Winklhofer, Sadat Nabi, McEnroe, Fabian |
| MCEC | Dubrovinsky, Kantor |
| BioCalc | Cuif, Dauphin |
| HydroMin | Winkler, Hermannsson, Wright, Ingrin, Bejina, Balan |
| ORION | Garcia |
| Grico | Deguen |
| Cubcat | Fernandez-Martinez |

In addition, several EuroMinSci collaborators participated, e.g. F. Bosi and N. Church (from MicroMagn) T. Balic-Zunic (associate to ORION) and G. Nehrke and M. Cussak (associated to BioCalc). There seems to have been a lack of communication within the CRPs to clarify that associated researchers could also be eligible for financial support.

A number of EuroMinSci participants were co-authors of oral or poster presentations, but did not attend. For example U. Halenius from MicroMagn or H. Skogby from HydroMin were co-authors of contributions. There is currently no mechanism to identify all EuroMinSci-related contributions.

3.2 Co-sponsoring of Session G 'Simulations of Earth and planetary materials: advances and limitations'

This session was explicitly named as being co-sponsored by the ESF EuroMinSci. That session was organized by E. Artacho (local organizer), B. Winkler (PL HydroMin) and E. Balan (PI in HydroMin). This was a full-day session, where six of the 16 oral contributions were given by EuroMinSci members. One keynote lecture was given by Julian Gale, who was invited by the ESF as an external expert.

It was gratifying to see that the medium sized-lecture hall was at all times slightly overcrowded, confirming that the interesting program had caught the attention of the general audience. It was also rewarding to see that a number of very high profile speakers (e.g. R. Cohen (Washington), D. Alfé (London) and M. Dove (Cambridge)) were keen to contribute. The UK MinSoc had requested that Michele Warren could give her lecture in that session in response to her being awarded with a research medal. This also shows that this session was seen as a high quality, attractive venue.

The scientific presentations clearly showed the immense progress atomistic modelling studies have made in the last years in the impact they have had and are still having in Mineral Sciences. The scientific scope was very broad, ranging from studies of molecules with surfaces to structure-property relations at extreme (pressure, temperature)-conditions. Specific highlights included the presentation by Lazerri on the computation of anharmonic properties, the key note lecture on extremely large scale simulations for crystal growth by J. Gale and the description of Metadynamics by A. Laio. M. Dove's keynote lecture on how 'cyberinformatics' will change the way science is done, in conjunction with insightful scientific results, was another outstanding contribution.

The poster session also demonstrated the use of atomistic simulations in all participating CRPs, as there were contributions from MCEC, MicroMagn, and HydroMin.

3.3. Co-sponsoring of Session H 'Mineral magnetism from the nanostructure to the planetary scale'

This session was also explicitly named as a session co-sponsored by the ESF EuroMinSci and was organized by Richard Harrison (PL MicroMagn) and J. Feinberg. It was a half-day session with eight oral presentations, five of which were given by EuroMinSci members and a further one given by the invited external expert J. Kischvink. Similarly, the poster session was dominated by EuroMinSci contributions, as five of the seven poster included EuroMinSci members.

The interesting aspect of this session was the link between quantum mechanical atomistic model simulations via empirical models and TEM investigations to large scale crustal features in mainly Norwegian rocks. The coherence with which the MicroMagn CRP presented itself was impressive. It was fascinating to see how a vast array of experimental approaches, including magnetic measurements, Mößbauer spectroscopy, and neutron scattering are combined with field observations in order to derive a coherent understanding of magnetism

from the atomistic to a macroscopic length scale. Undoubtedly, this session conveyed the intent of MicroMagn to a wide audience and was an excellent display of the synergies due to European-wide funding of a combined modeling-experimental-field work study.

The external expert, J Kirschvink, gave a overview over the use of ferromagnetic resonance spectroscopy to identify samples of bacterial magnetofossils useful for further studies by SEM or TEM. This clearly is an evolving field of research with a notable potential.

3.4 Other sessions

EuroMinSci members presented their science also in other sessions. For example, J. Ingrin (HydroMin) gave a talk in session U 'Volatiles in Minerals and their petrologic implications', R. Deguen from the Grico CRP described their experimental set-up in session J 'Mineralogy, structure and dynamics of the Earth's mantle' and K. Wright (HydroMin) was co-author of a presentation in the session M 'Amorphous materials'.

3.4 Feed-back

I talked to nearly all EuroMinSci members at the meeting. There was a general consensus that the meeting was of very high standard, and that this had been an excellent opportunity to present and discuss the science done in the EuroMinSci framework. It was after this meeting that a consensus emerged that e.g. Norwegian associates will begin to lobby their funding agency to support a extension / prolongation of EuroMinSci. The written comments after the meeting were unanimously positive. The feed-back and comments from scientists not involved in EuroMinSci were equally positive. EuroMinSci was perceived as a first-rate scientific collaboration.

4. Budget

The total contribution by the ESF towards this networking activity was

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| travel, conference participation, subsistence of EuroMinSci members | 16.914 € |
| external experts | 3.000 € |
| local organization /co-sponsorship of the conference | 2.200 € |
| Sum | 22.114 € |

This sum is significantly less than anticipated. There are two reasons for this

(a) There were only 20 participants instead of 27

(b) Flights were significantly less expensive than anticipated. We estimated 450 €per participant, but average flight costs were 200 €, and five participants did not claim flight costs.

5. Final conclusions and recommendations

The funding of networking activities in order to further the scientific collaborations between CRPs is a corner-stone of the EUROCORES concept. The co-sponsoring of the Frontier meeting was such as cross-CRP activity and it undoubtedly was a real success. Clearly, EuroMinSci presented itself to the relevant international community and demonstrated that it produces first class science.

The procedure to apply and support networking activity is seen as very efficient.

The flexibility in terms of adapting the budget of networking activities to changes in number of participation / costs was really helpful.

The planning started on the understanding that the ratio of funding for external to internal speakers should be approximately 10%. In the present case it was 14% . The recommendation here is that a band of 10 - 20% seems more appropriate, and that 10% is probably a lower bound, as 2 external speakers for 20 participants seems very reasonable.

Procedures for reimbursement through the organizer of a network should probably be changed. It took us more than six months to reimburse everybody. Probably a reimbursement directly through the ESF, which is more experienced with international reimbursements, is more efficient.