

**Proposal for a CECAM/Psi-k workshop:**

**Multiscale modeling of cohesion and structure of extended defects  
in metallic materials**

**Organizers:**

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**Dates and length:**

We plan to organize this workshop in CECAM for three full days, preferably in the period of June 17--19, or June 26--28, 2006.

**Motivation and objectives**

Exploring connections between macroscopic characteristics of materials and their microscopic structure in atomistic dimensions has been an important topic in contemporary solid-state physics and materials science. A better understanding of the relations between macroscopic properties of solids and their structure yields new knowledge needed for development of materials with better technological properties.

Extended defects, such as grain boundaries, stacking faults, antiphase boundaries and interphase boundaries in multiphase materials are important elements of microstructure in polycrystalline solids, which have been widely used as engineering materials. They determine to a large extent many of the properties of polycrystalline materials and play an important role as preferential sites in most metallurgical processes. Numerous studies of the structure and properties of these defects revealed that their physical, chemical and mechanical properties strongly depend on their type and crystallographic orientation.

Recently, theoretical calculations regarding atomic configuration and properties of extended defects in materials became possible using ab initio ES calculations, i.e. fundamental quantum theory (Schrödinger equation). Here the atomic numbers of constituent atoms and some structural information are employed as the only input data. Such calculations are routinely performed within the framework of density functional theory in which the complicated many-body interaction of all electrons is replaced by an equivalent but simpler problem of a single electron moving in an effective potential. For a given material, the

calculated total energies are used to obtain equilibrium lattice parameters, elastic moduli, relative stabilities of competing crystal structures, energies associated with point and planar defects, alloy heat formations, etc. In addition, we also obtain information about electronic densities of states and charge densities that enable us to attain a deeper insight and learn which aspects of the problem are important. For internal interfaces and other defects, these calculations are computationally very demanding and, therefore, at the beginning, only simple interfaces were treated.

The aim of the proposed workshop is to bring together representatives of solid-state physics and metallurgy communities to present and discuss state-of-the-art developments and perspectives of solid-state, computational and molecular physics techniques in modelling of cohesion and structure of extended defects in materials. Studies of the influence of extended defects on the properties of materials are a high priority in the research agenda of world leading academic and industrial laboratories. Knowledge of processes occurring in condensed matter at atomistic and electronic level contributes to deep understanding of technologically important properties and to developing new materials. Our proposal perfectly fits into this trend.

### **Format**

In total we wish to have approximately 45 participants, including about 5 experimentalists and at least 10 junior scientists. We intend to invite on one side physicists representing leading research groups in state of the art applications of DFT, Monte Carlo, and other techniques, but also to attract young researchers to present their work. During 3 days of the workshop there will be 15-18 review talks (45-50 minutes plus 15-10 minutes discussion) and several short presentations (20 minutes) of younger researchers from different groups.

### **Budget**

We estimate the cost per participant (excluding travel to Lyon) to be 250 EUR. This includes meals and accommodation for three nights in Lyon (assuming 10 junior participants staying in the ENS hostel).

We would like to provide full support for invited speakers and participants. This gives 11250 EUR. Also we plan to support travel costs of some speakers, which adds 4500 EUR to the budget giving in total 15750 EUR.

We are thus requesting 7750 EUR from CECAM and 8000 EUR from Psi-k.

### **References**

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## Support

Additional funds beyond this specified above would allow us to offer support of travel expenses to junior participants. We plan to apply for this to COST P-19 action.

The suggested list of speakers includes several from the US and Japan and the cover of their travel costs (to be sought from CECAM) is included in the above budget.

We plan to contact potential speakers soon and will investigate the possibility of accessing some of the funds suggested in the call for proposals.

## Preliminary list of participants

I. Abrikosov, S  
 H. Dreysse, F  
 C. Elsaesser, D  
 M. W. Finnis, UK  
 A. J. Freeman, Northwestern University, USA  
 J. Hafner, Vienna, Austria  
 T. Kitamura, Kyoto Univ., Japan  
 P. Lejcek, CZ  
 W. Lojkowski, Warsaw, PL  
 S. Mueller, Erlangen, D  
 J. Neugebauer, D  
 R.M. Nieminen, FIN  
 V. Paidar, CZ  
 D. G. Pettifor, Oxford, UK  
 M. Scheffler, D  
 B. Smit, CECAM, F  
 D. Srolowitz, USA  
 A.P. Sutton, UK  
 V. Vitek, University of Pennsylvania, USA  
 G. Wahnstrom, Chalmers University, Gothenburg, S  
 D. Wolf, USA  
 C. Wolverton, USA  
 S. Yip, USA  
 A. Zunger, USA