

Multiscale approach to alloys: advances and challenges

Organizers:

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Motivation:

The dominating approach in studying materials is experiments. At the same time, rapid progress is taking place in the field of numerical computations. This put on the agenda the idea of *ab initio* design of structural materials, most of which are alloys. However, it is important to understand that conventional electronic structure calculations in the framework of the DFT predict materials properties in the ground state, that is at temperature $T=0\text{K}$. There are schemes that allow one to consider the effect of nonzero temperature, the most famous example here would be *ab initio* molecular dynamics. Unfortunately, the scheme is very demanding in terms of computational resources, and at present covers rather limited time and length scales.

An alternative approach that leads to a successful description of alloys is given in the framework of the so-called multiscale modelling. By this one understands a solution of the complete problem step-by-step employing theoretical methodologies, which are suitable for the particular length and/or time scale followed by an appropriate coarse graining when proceeding towards the next (larger) scale. For example, one starts with the solution of the quantum mechanical problem within DFT for a relatively small system (~ 100 atoms). From these results one determines interactions between different atoms and uses them in simulations (classical molecular dynamics or statistical mechanics, e.g. Monte-Carlo technique), which includes 10^3 to 10^5 particles. In doing so one can study, for example, crack propagations, melting, or ordering in metals and alloys. For simulations of mechanical properties and microstructure (i.e. properties on the scale of microns) one often needs to substitute the atomistic description by continuum theories. The latter can be done, for example, in the framework of the phase-field model.

The goal of the conference is to bring together leading experts working in the field of multiscale modeling for alloys, and to exchange the expertise on the recent advantages in the field, as well as to discuss challenges on the way to the development of a consistent set of tools for *ab initio* simulations of disordered materials at all levels, from the electronic structure towards the microstructure.

In addition, we will invite leading experimentalists in the fields of spectroscopy, nanoscience, structural chemistry, and geophysics, to establish closer links between theory and experiment. In doing so we will also attract additional support for the conference, e.g. from EuroMinSci ESF program, as well as important national programs (USA, Sweden, etc.).

Time and place:

A three-four day workshop is scheduled for June-July 2007 in Sweden, Stockholm region.

Participants:

We will bring together leading experts, representing different schools (often with very opposite views) in the field, and also covering all the aspects of the multiscale modeling. It is important that they represent academia, as well as industry, theory and experiment. Tentative list of speakers include:

Prof. C. Wolverton (Ford Motor Company, USA)
Prof. G. Ceder (MIT, USA)
Prof. B. Johansson (KTH, Sweden, and Sandvik Steel)
Prof. I. A. Abrikosov (Linköping, Sweden)
Prof. H. Dryesse (Strasbourg, France)
Prof. Yu. Kh. Vekilov (Moscow, Russia)
Prof. M. Katsnelson (Nijmegen, The Netherlands)
Prof. A. V. Ruban (KTH, Sweden)
Prof. M. Asta (Chicago, USA)
Prof. G. M. Stocks (Oak Ridge National Laboratory, USA)
Prof. A. Zunger (NREL, USA)
Prof. H. Skriver (DTU, Denmark)
Prof. L. Vitos (Budapest, Hungary and Stockholm, Sweden)
Prof. J. Kollar (Budapest, Hungary)
Prof. B. Gyorffy (UK)
Prof. P. Weightman (University of Liverpool)
Prof. S. Lidin (Stockholm, Sweden)
Prof. L. Dubrovinskii (Bayreuth, Germany)
Prof. R. Zeller (Juelich, Germany)
Prof. J. Neugebauer (Max-Planck-Institute, Dusseldorf, Germany)

In addition, we will encourage and support financially participation of young researchers and PhD students. Total number of participants is expected to be around 35.

Participants:

Preliminary negotiations with conference centers in Sweden indicate that a cost for accommodation (including full board) will be around 150 Euro per person per day. Travel support will be needed, especially for participants from US and young researchers, about 10000 Euro. Additional funding will be requested from the Swedish Research Council, and the Royal Swedish Academy of Sciences. We thus request a support of 10000 Euro from Psi-k.

CURRICULUM VITAE FOR IGOR ABRIKOSOV

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- Personal** Born October 15, 1965; Married, 3 children;
Citizenship: Sweden, Russia
- Professional preparation** Master of science examination in "Physics of Metals" at Moscow Steel & Alloys Institute, Moscow, Russia, 1988, "excellent" grade;
Candidate of Physical and Mathematical Science in "Solid State Physics", Moscow Steel & Alloys Institute, Moscow, Russia, 1991;
Doctor of Physics and Mathematics in "Solid State Physics", Moscow Steel & Alloys Institute, Moscow, Russia, 1997;
Docent in "Condensed Matter Physics" at Uppsala University, Sweden, 1997.
- Appointments** Professor, Theoretical Physics, Department of Physics and Measurement Technology, Linköping University, Sweden, 2003- present time;
Senior Researcher, Swedish Research Council and Associate Professor, Condensed Matter Theory Group, Uppsala University, Sweden, 1999 - 2003;
Assistant Professor, Condensed Matter Theory Group, Uppsala University, Sweden, 1995 - 1999;
Visiting Scientist, Condensed Matter Theory Group, Uppsala University, Sweden, 1993 - 1995;
Visiting Scientist, Physics Department, Technical University of Denmark, Denmark, 1992 - 1993.
- Commissions of trust and administration** Head of the Theory and Modeling Division at the Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden, September, 2003 - present time;
Spokesperson for Working Group 15 "Ab initio design of structural materials" within ESF Programme "Towards Atomistic Materials Design (Psi-k)", 2002-present time;
Project Leader for EuroMinSci Programme "Mineralogy and Chemistry of Earth's core" from the European Science Foundation (ESF), starting in 2006;
Board member, Center for Nanotechnology, (CeNano), Linköping University, Sweden, October, 2003 - present time;
Coordinator for interuniversity international cooperation at the Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden, May 2004 - present time;
Acting head of the Condensed Matter Theory Group (Fysik IV), Department of Physics, Uppsala University, 2002-2003;
Reviewer of scientific papers for 9 international journals;
Reviewer of research applications for the US Department of Energy;
Reviewer of applications for the European Science Foundation;
Reviewer of applications for the Swedish Research Council (VR);
Reviewer of applications for The Royal Swedish Academy of Sciences (KVA).

Supervision, PhD students	<p>Dr. Leonid V. Pourovskii (PhD in 2003, at present Postdoctoral Fellow, Ecole Polytechnique, Paris, France).</p> <p>Weine Olovsson (PhD in 2005, currently Postdoctoral Fellow, Stockholm University, Sweden).</p> <p>Principal supervisor for A. Kissavos (2001 –).</p> <p>Principal supervisor for F. Liot (2002 –).</p> <p>Principal supervisor for C. Göransson (2005-).</p> <p>Principal supervisor for T. Martin (2005-).</p> <p>Principal supervisor for B. Alling (2005-).</p> <p>Supervisor for Marie Curie Training Site Fellows S. Schallcross (PhD in 2003) and L. Chioncel (PhD in 2004).</p> <p>Co-supervisor of 5 PhD students.</p>
Networks in academia and industry	<p>SSF INGVAR Network</p> <p>SSF material consortium "Inalloy"</p> <p>ESF Program "Towards Atomistic Materials Design (Psi-k)"</p> <p>EuroMinSci Eurocore program "Mineralogy and Chemistry of Earth's core" (ESF)</p>
Awards	<p>Distinguished M.Sc. Diploma (1988);</p> <p>Junior Individual Grant from SSF(1998);</p> <p>Oscar prize (2000);</p> <p>Individual Grant for the Advancement of Research Leaders from SSF (INGVAR grant, 2001).</p>
Selected invited presentations	<p>Invited presentations at <u>23 international conferences</u> (1 Plenary).</p> <p>Psi-k Conferences, Schwäbisch Gmünd, Germany, 1996, 2000, and 2005;</p> <p>Annual Meetings & Exhibitions of the Minerals, Metals & Materials Society, USA, 2001, 2002, and 2005;</p> <p>American Physical Society (APS) March Meeting 2004;</p> <p>5th international Ringberg-Workshop on Thermodynamic Modelling and First-Principle Calculations, Schloss Ringberg, Germany, 2005 (Plenary).</p>
Organized workshops	<p>Workshop on applications of LMTO method, Uppsala, Sweden, 2000;</p> <p>International Conference on Electronic Structure Theory, Uppsala, Sweden, June, 2002;</p> <p>INGVAR scientific Workshop, Hasseludden, Sweden, 2003;</p> <p><i>Ab initio</i> design of structural materials, Uppsala, Sweden, 2003;</p> <p>2nd International Symposium On Hydrogen In Matter, Uppsala, Sweden, 2005;</p> <p>Symposium M: Alloys: theory and applications to structural materials at Psi-k2005 Conference, Schwäbisch Gmünd, Germany, 2005.</p>
Teaching	<p>Lecture course "Statistical Mechanics" for undergraduate students;</p> <p>Several courses in condensed matter theory for undergraduate and postgraduate students;</p> <p>Invited tutorial Quantum Simulation of Liquids and Solids at Centre Européen de Calcul Atomique et Moléculaire (CECAM, France 2005).</p>
Entrepreneurial achievements	<p>New computer cluster for physical computations built in collaboration with National Supercomputer Centre in Linköping.</p>

5 SELECTED PUBLICATIONS FOR PROF. IGOR ABRIKOSOV

1. L. Dubrovinsky, N. Dubrovinskaia, F. Langenhorst, D. Dobson, D. Rubie, C. Geshmann, I. A. Abrikosov, B. Johansson, V. I. Baykov, L. Vitos, T. Le Bihan, W. A. Crichton, V. Dmitriev, and H.-P. Weber, "Iron-silica interaction at extreme conditions and the electrically conducting layer at the base of Earth's mantle", *Nature* **422**, 58 (2003), www.nature.com
2. W. Olovsson, I. A. Abrikosov, B. Johansson, A. Newton, R. J. Cole, and P. Weightman, "Auger energy shifts in fcc AgPd random alloys from complete screening picture and experiment", *Phys. Rev. Lett.* **92**, 226406 (2004), <http://publish.aps.org/>
3. J. Hunter Dunn, O. Karis, D. Arvanitis, R. Carr, I. A. Abrikosov, B. Sanyal, L. Bergqvist, and O. Eriksson, "Vanishing magnetic interactions in ferromagnetic thin films", *Phys. Rev. Lett.* **94**, 217202 (2005), <http://publish.aps.org/>
4. L. Dubrovinsky, N. Dubrovinskaia, I. Kantor, W. A. Crichton, V. Dmitriev, V. Prakapenka, G. Shen, L. Vitos, R. Ahuja, B. Johansson, and I. A. Abrikosov, "Beating the miscibility barrier between iron and magnesium by high-pressure alloying", *Phys. Rev. Lett.* **95**, 245502 (2005), <http://publish.aps.org/>
5. D. A. Andersson, S. I. Simak, N. V. Skorodumova, I. A. Abrikosov, and B. Johansson, "Optimization of ionic conductivity in doped ceria", *PNAS* **103**, 3518 (2006)