Scientific report on the workshop
"Multiscale approach to alloys: advances and challenges"
June 17-19, 2007, Stockholm/Sigtuna Sweden

Summary.

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* materials design, presented in details at the conference in several talks in relation to materials for modern electronic, dilute magnetic semiconductors, hydrogen storage materials, and fast ion conductors for fuel cell applications. It is also 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=0K. 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. **The goal of the workshop was to bring together leading experts, theoretician and experimentalists, 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.**

The workshop was organized by Prof. Igor A. Abrikosov (Linköpings University, Sweden), Prof. H. Dreysse (Universite Louis Pasteur, Strasbourg Cedex, France), Prof. G. Ceder (Massachusetts Institute of Tecnology, USA), Prof. M. Asta (UC Davis, USA), and Prof. L. Dubrovinsky (Universität Bayreuth, Germany). It took place at Sigtunahöjden Conference Center, attracted 60 participants from 16 countries, representing Europe, USA, Japan, India, and China. The workshop was composed of nine oral sessions with 27 Invited Presentation, given by the leading scientists in the field, and two poster sessions with 28 presentations.

We would like to acknowledge the support to the conference which is received from the European Science Foundation Network "Towards Atomistic Materials Design (Psi-k)" (http://psik.dl.ac.uk), the Swedish Research Council (http://www.vr.se), the Strategic Research Center MS^2E at Linköping University (http://www.liu.se/ms2e), Materials Science Consortium "Inalloy" from the Swedish Foundation for Strategic Research (http://www.stratresearch.se/), and European Science Foundation COST action P19 (http://www.cost.esf.org/). This event has been made possible thanks to the support from the European Science Foundation (ESF) under the EUROCORES Programme EuroMinScI (www.esf.org/eurominsci), through contract No.ERAS-CT-2003-980409 of the European Commission, DG Research, FP6.

Scientific content of the event.

The workshop covered fundamental issues within the alloy theory, such as development of novel methodologies for *ab initio* simulations of alloys, multiscale approach to alloys thermodynamics, kinetics, and magnetism, properties of low-dimensional and nanoscale systems, and behavior of alloy phases at extreme conditions. Several presentations were devoted to the description of advantages in experimental studies of alloys. New fields for applications of the alloy theory have been discussed. Special emphasis here has been given to theoretical predictions of novel phases relevant for energy applications, geophysical community, metallurgy, and electronics. The topics covered are simulations of metallic and semiconductor alloys, magnetic materials, hard materials, hydrides and oxides.

The scientific topics discussed during the workshop can be divided into several mutually related areas:

Simulations of alloys: from the electronic structure towards large-scale simulations. **Levente Vitos** described recently developed Exact Muffin-Tin Orbitals (EMTO) method in combination with the Coherent Potential Approximation (CPA). In his talk he presented the main characteristics of the EMTO-CPA method, and demonstrated it through a few applications for simple and transition metal alloys. **Duane D. Johnson** showed in his talk that one can starting from Schrödinger's equation make quantitative prediction of onset twinning stress in elements and alloys. Deformation twinning is observed in numerous engineering, chemical, and geological materials. Yet, unlike for shearing, there is no fundamental yield-stress criterion for twinning. Duane Johnson resolved this long-standing issue.

Alloys at extreme conditions. **Leonid Dubrovinsky** presented experimental evidences for body-centered-cubic phase of iron-nickel alloy in the Earth's core. He studied the iron-nickel alloy Fe0.9Ni0.1 in situ by means of the angle dispersive X-ray diffraction in internally heated diamond anvil cells (DACs) and measured its resistance as a function of pressure and temperature. He found that at pressures above 225 GPa and temperatures over 3400 K Fe0.9Ni0.1 adopts the bcc structure. The new experimental and theoretical results suggest that iron alloys with geochemically reasonable compositions (e.g. with significant nickel, sulfur, or silicon content) adopt the bcc-structure in the Earth's inner core. **Dane Morgan** used first-principles based thermodynamic modeling to calculate the energetics and spin crossover properties of $(Mg,Fe,Al)(Si,Al)O_3$ perovskite and (Mg,Fe)O ferropericlase under the extreme pressures and temperatures of the lower mantle, and found a strong dependence of the spin crossover on composition and structure, including opposite compositional trends for perovskite compared to ferropericlase. These differences in turn couple strongly to the phase stability and Fe partitioning. **Victor Vinograd** studied thermodynamics of mixing in complex oxides based on force-field models. He used the cluster expansion method of Connolly and Williams, followed by Monte Carlo simulations of the effects of mixing and ordering in some geologically important materials. The accuracy of the force-field model used by Victor Vinograd were tested by comparing the predicted excess energies of a limited set of configurations with those calculated *ab initio*.

Multiscale approach to alloys thermodynamics, kinetics and magnetism. **Alex Zunger** put forward the inverse design problem, that is to find the atomic configuration with a desired target physical property. He focused on the calculation of the electronic and magnetic consequences of the structure at (x,T). This approach has two different realizations. In the first one he took the microstructure predicted from our Mixed Basis Cluster Expansion plus Monte Carlo simulation and feed it into a supercell calculation of the electronic and magnetic properties. In the second version (Inverse Band Structure) he ignored thermodynamics and search automatically (via genetic algorithms) which ordered or disordered atomic arrangement on a lattice had a given electronic property. **Axel van de Walle** presented recent additions to the Alloy Theoretic Automated Toolkit (ATAT). This is a software package automating the construction and the simulation of lattice-gas models based upon *ab initio* data that is aimed at generating quantitative thermodynamic data for solid-state alloy systems. Recent progress in the development of this software package were presented. **Anton Van der Ven** emphasized that alloys and complex oxides were often characterized by differing degrees of short and long-range order. This affects not only activation barriers, which vary with local order, but also leads to important correlations between successive hops of diffusing atoms. He described how diffusion coefficients can be calculated from first-principles in non-dilute multi-component solids in which the role of short and long-range order was explicitly accounted for. The approach relied on the evaluation of Kubo-Green expressions, which provide the link between macroscopic diffusion coefficients and atomic trajectories sampled in kinetic Monte Carlo simulations. **G. Malcolm Stocks** pointed out that the ability to perform large scale first-principles calculations enabled the study of the magnetic state of complex materials without the need to make *de novo* assumptions regarding the expected magnetic order. In the presentation Malcolm Stocks reviewed some of his recent studies of the magnetic structure of such complex systems using state of the art surface embedding and order-*N* multiple scattering Green's function methods. **Balazs Gyorffy** described and advocated the construction of First-Principles Landau Theories based on the KKR-CPA methodology for describing phase diagrams of alloys. The essence of the idea was to calculate the coefficients in the Landau expansion of the free energy, from first principles directly without an intermediate step involving statistical mechanical calculations based on effective Hamiltonians, as properties of the high temperature high symmetry phase. This way of proceeding was contrasted with the conventional alternative which starts with ground state searches and ground state calculations and then includes thermal fluctuations which eventually, at some transition temperature T_c , destroys long range order. **Andrej Ruban** demonstrated the impact of magnetism upon chemical interactions in alloys. The effect was discussed on the basis of ordering behavior in such systems as fcc Fe-Ni, bcc Fe-Cr, and fcc Fe-Cr-Ni alloys. The results were obtained by the generalized perturbation method and in total energy calculations in the framework of density functional theory.

Surface alloys, low-dimensional and nanoscale systems. **Bernd Schönfeld** presented his diffuse scattering studies of bulk and near-surface microstructure of alloys. The local atomic arrangement of binary alloys has been repeatedly analysed from x-ray and neutron scattering. While local order at elevated temperature and the evaluation of effective pair interaction parameters for states of thermal equilibrium were the domain of neutron

scattering, the strength of x-rays lied in the determination of the species-dependent atomic displacements. Here the 3λ-method allowed the achievable precision to be assessed. Results from in-plane scattering of the Pt-Rh (110) and (111) surfaces performed at the Swiss Light Source, were presented. It was found that the microstructure depends on the type of surface. **Harald Reichert** concentrated on fluctuations in binary alloys. The experimental investigation of such fluctuations on a microscopic length scale presented a formidable challenge as they were dynamic in nature. As an example the static part of the fluctuation spectrum in the binary system Cu3Au and in FeCo thin films were discussed. Moreover, with the refinement of experimental tools and the advent of powerful sources of x-rays and electrons time-resolved studies of fluctuations have become possible. Two recent experimental results on the behaviour of fluctuations in a critical system (Fe3Al) as well as a noncritical system (Cu3Au) were discussed in detail. **Micha Polak** extracted coordination-dependent bond-energy variations from surface-energy anisotropies for the study of alloy nanocluster surface properties. Using his free-energy concentration expansion method, he was able to explore compositional structures and properties of binary and ternary nanoclusters in Rh-Pt-Pd system. **Hugues Dreysse** presented his study of equilibrium size distribution of 1D surface clusters. He proposed an atomistic model for the submonolayer growth with elastic and chemical interactions being taken into account. By assuming a coherent deposition, the system was projected onto a lattice gas model in a way similar to cluster expansion in the alloy theory. The 1D case has been solved exactly. Extensions to 2D and 3D growth were also discussed. **Dario Alfe** presented a technique for computing by first-principles simulation the chemical potential of adsorbate molecules on a surface for any coverage and temperature. The technique is capable of giving absolute values for the frequency prefactor appearing in the Polanyi-Wigner formula for the desorption rate. It was applied to the case of H_2O on the MgO (001) surface at low coverage. **Matti Alatalo** have studied the adsorption of O2 on Cu(100) using *ab initio* molecular dynamics and static potential energy surface calculations. He discussed the role of surface phonons in the dissociation process of O2 at low incident energies, and showed that the phonons affect the dissociation by creating structures that resemble those of the (110) surface rather than by transferring enough energy to the molecule to dissociate. **Mark Asta** studied nanometer-scale phase separation in bulk immiscible Fe-Ag alloys, deposited as epitaxial thin films on Mo(110) and Ru(0001) substrates. A hybrid atomic-scale/contiunuum theoretical model was proposed to elucidate the competition between elastic and chemical interactions underlying the thermodynamic stability of these structures. Implications of this work for achieving highly ordered stripe patterns was discussed.

Applications. This included studies of nitrides, semiconductor alloys, hydrides, oxides, and steels. **Sandro Scandolo** presented his results for PtN2 and OsN2, which belong to a new family of nitrides synthesized recently at high pressures from their parent elements. The compounds have bulk moduli comparable with those of the traditional superhard materials. Their crystal structures -pyrite for PtN2 and marcasite for OsN2- have been determined by comparing the results of *ab-initio* calculations with x-ray, Raman, and compressibility measurements. A comparison between their formation energies explained the similar thermodynamic conditions of formation reported experimentally for the two compounds. **Joerg Neugebauer** shed some light on the intricate interplay between

kinetically driven stabilization of alloy structures in Group-III-nitride alloys ((In-Ga)N, (Al-Ga)N and diluted nitrides (Ga(As-N), (In-Ga)(As-N)) at the surface and in the bulk and employed a DFT-based set of tools to (i) identify the thermodynamically stable surfaces under realistic growth conditions, (ii) determine/quantify the relevant kinetic processes (adatom diffusion, desorption, nucleation) on these surfaces, and based on these atomistic information determine (iii) growth morphology and chemical order employing statistical approaches (kMC). **Pavel Korzhavyi** described results of his systematic studies of the magnetic and chemical ordering trends of 3*d* transition metal (TM) impurities in the GaAs and ZnO hosts are performed using *ab initio* calculations. Two approaches, the one based on the coherent potential approximation and the other employing supercell calculations, yielded similar results for the magnetic moments as well as for the energies of magnetic ordering. **Chris Wolverton** presented results from an effort he has been developing over the past few years directed a predicting novel hydrogen storage materials from a computational first-principles approach. Chris Wolverton showed examples of progress he has made in three areas: (i) prediction of hydriding enthalpies and free energies across a wide range of hydride materials, (ii) prediction of crystal structures for multivalent alanates and borohydrides, [such as Ca(AlH4)2 and Ca(BH4)2], and (iii) predicted decomposition pathways for Li4BN3H10 and destabilized systems based on combinations of LiBH4, Ca(BH4)2 and metal hydrides. **Sergei Simak** emphasized that ceria (CeO2) is known for its ability to easily store, release, and transport oxygen. Therefore it is an attractive material for oxygen storage and fuel cell applications. He showed from first principles how useful macroscopic properties of doped ceria correlate with its properties at the atomic level. **Ben Burton** performed molecular dynamics simulations on a first-principles-based effective Hamiltonians for chemically short-range ordered Pb(Sc0.5Nb0.5)O3 with nearest neighbor [Pb-O] divacancy pairs. The divacancy-concentration (X[Pb-O]) vs. temperature phase diagram was calculated. Similar calculations have been performed for a chemically random system and one with ideal NaCl-type Sc:Nb order. **Börje Johansson** and **Levente Vitos** presented an insight into the electronic and magnetic structure, micro-mechanical, and surface properties of austenitic stainless steels. **Marcel Sluiter** in his talk outlined the application of alloy theory to complex carbides relevant to low alloyed steel. The unifying features of a variety of seemingly unrelated structures were discussed with regard to phase stability. Some implications of processes on the atomic scale on material properties on a macroscopic scale were discussed as well. **Adam Kiejna** studied the effect of impurity chromium atoms placed in interstitial and substitutional positions at symmetric Sigma 5(210) grain boundary in bcc iron. Full relaxation of supercell shape and volume was applied which resulted in stable asymmetric grain boundaries, with the grains shifted with respect to each other. Energetics of the grain boundary cohesion and segregation, as well as the magnetic properties of the system were presented.

All the oral presentations were followed by useful discussions, which continued during breaks and poster sessions. A complete book of abstracts, which also include all the poster abstracts, is posted at the conference web-site
http://cms.ifm.liu.se/theomod/theophys/intl._alloy_conference/

Assessment of the results and impact of the event on the future direction of the field.

The workshop participants agreed that the electronic density functional theory is making a tremendous impact in the modelling of materials. Increasingly, parameters that once were accessible exclusively through experimentation are now with much less cost and effort computed. Since the eighties it has been possible to predict crystal structures and lattice parameters of the most commonly occurring metallic materials. It was quickly realized that through calculation of the total energy of alloy phases, the thermodynamics of alloys could be predicted and phase diagrams could be computed. Gradually not just perfect crystals, but defects also could be treated.

However, many of the early applications of this new methodology for alloy phase stability were focused on alloys based on metals such as aluminum that are relatively easy to handle theoretically. Until recently, more complex systems, like alloys based on iron, disordered oxides and nitrides, and semiconductor alloys received scant attention due to the great importance of hard to handle elements such as carbon and nitrogen, and because of the complications associated with magnetism. The multiscale modelling allowed for a tremendous progress within the field. 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. A success of the approach, illustrated in many talks and posters during the workshop, put on the agenda a possibility of *ab initio* materials design. Alex Zunger said that this is a new style of doing business in alloy theory, resulting in new types of predictions which he illustrated in his talk.

As a matter of fact, the participants put lot of attention to challenges within the field. Chris Wolverton emphasized that such an approach requires several key capabilities: (i) Accurate prediction of thermodynamic properties for the electronic ground state, (ii) Prediction of crystal structures for unknown materials, and (iii) Prediction of preferred decomposition pathways. The field still needs to put efforts into methodological developments within the multiscale modeling. Dario Alfe pointed out that comparisons with experiment provide an important test of the accuracy of the simulations. But to probe the accuracy of the calculations in more detail, we should follow advances in rapidly developing many-body theory. For example, he presented tests of the accuracy of the generalised gradient form of exchange-correlation energy for his system via calculations by using quantum Monte Carlo method.

In summary, we believe that the future development of our filed should proceed along two principal directions: (i) competence development and (ii) competence transfer. The former direction includes the following problems:

1. Complexity. There are increasing demands in theoretical understanding of more and more realistic materials (including materials for nano-science, amorphous phases, quasicrystals, non-commensurate structures, alloy surfaces, etc.) and materials phenomena (radiation damage, hydrogen storage, ion conductivity, brittleness, hardness). Increasing length scale for the simulations requires a development of novel, more efficient techniques for solving the electronic structure problem *within* LDA-GGA DFT.
2. Temperature: From the total energy towards the free energy. A majority of applications still involve simulations at T=0K. We have to develop efficient and reliable tools for

simulations at elevated temperature that include the effect of lattice vibrations, schemes for calculations of elastic constants and phonons in alloys, and for carrying out *ab initio* molecular dynamics for alloys. Here the fundamental problem is to treat *simultaneously* configurational and vibrational contributions to the free energy, besides extraordinary demands for the computer power. Development of reliable quasi *ab initio* approaches shall continue as well.

3. Strong electron correlations. Here we see our role as to extending applications of novel many-body techniques to realistic materials of technological importance. This will substantially enhance capabilities of the alloy theory to treat materials important for e.g. electronic applications, semiconductor alloys, fuel cell, batteries materials, light emission and light detection processes, and transport.

4. Complex magnetism. Most of the modern structural materials are Fe-based alloys. It has recently become clear that complex magnetism of Fe substantially influence properties of these materials. We must develop techniques, which allows for the simulations of materials with complex crystal and magnetic structures. It is worth mentioning that *almost all* classical MD simulations for the moment *ignore* magnetism.

The competence transfer also faces many challenges. A distribution of computer codes for the electronic structure calculations goes much faster than the transfer of the corresponding knowledge for the underlying theory. Unfortunately, though the codes have become really user friendly, the theory on its own has not. Therefore using the codes is not fool proof, which is a real danger for the field, in two ways. Firstly, funding agencies may stop to considering the field as a part of science, and developmental work has increasingly harder time to motivate the needs for support. Secondly, errors produced by non-experienced users, as well as their unmotivated high expectations, may accumulate, and create overall negative impression for the possibilities of the theory. We see a real and clear necessity to educate, at substantially increased rate, highly qualified experts in the field. We need to switch a paradigm here, and complement the training of *individuals* (individual PhD students and Postdoctoral Fellows carrying out their projects with leading Professors) by the *general training for the wide community of users of ab initio simulation tools.* For this, the following actions need to be taken.

- Building of European Network for the Transfer of Knowledge that should coordinate and organize different kinds of training activities: tutorials, summer schools, etc.
- Setting up and financing Competence Centers around leading teams in the field capable to providing long term (from one month up to half-year) training for graduate students and postdoctoral fellows, organized in groups. Making the know-how accumulated by the experts available for the users. Organizing internet forums, newsletters (perhaps, based on Psi-k newsletter), etc.
- Maintain a possibility of organizing major conferences in the field on a regular basis. Tradition of Psi-k Schwäbisch Gmünd conferences is essential for our future.
- Getting the electronic structure theory on the list of undergraduate courses.

Very many participants pointed out that the workshop was extremely successful from scientific point of view, and was very well organized.

Scientific program:

Sunday, June 17
12.00 – 14.00 Registration and lunch

14.00 - 14.30 Welcome (conference organizers)

Session I. Simulations of alloys: from the electronic structure towards large-scale simulations

Chair: H. Dreysse

14.30 – 15.00 Levente Vitos (Royal Institute of Technology, Sweden), "The Exact Muffin-Tin Orbitals-CPA Method and Applications"
15.00 - 15.30 Duane Johnson (University of Illinois Urbana-Champaign, USA), "From Schrödinger's Equation to the Rolling Mill: Quantitative Prediction of Onset Twinning Stress in Elements and Alloys"

15.30-16.00 Coffee break

Session II. Alloys at extreme conditions.

Chair: S. I. Simak

16.00 – 16.30 Leonid Dubrovinsky (University of Bayreuth, Germany), "Experimental Evidences for Body-Centred-Cubic Phase of Iron-Nickel Alloy in the Earth's Core"
16.30 – 17.00 Dane Morgan (University of Wisconsin, USA), "First-Principles Study of Fe and Lower Mantle Phase Stability"
17.00 – 17.30 Ricardo Grau-Crespo (University College London, UK), "Symmetry-adapted configurational modelling of fractional site-occupancy in solids: introduction to the SOD program"
17.30 -18.00 Victor Vinograd (University of Frankfurt, Germany), "Thermodynamics of mixing in complex oxides based on force-field models"

18.00 - 19.00 **Poster session I**

19.00-20.30 Dinner

20.30- **Poster session I**

Monday, June 18

Session III. Multiscale approach to alloys thermodynamics and kinetics

Chair: L. Vitos

9.00 – 9.30 Alex Zunger (NREL, USA), "The Invers Design Problem : Find the atomic configuration with a desired target physical property"
9.30 – 10.00 Axel van de Walle (Cal Tech, USA), “Recent additions to the Alloy Theoretic Automated Toolkit”
10.00 – 10.30 Anton Van der Ven (University of Michigan, USA) “First-principles prediction of diffusion coefficients in non-dilute, multi-component solids”

10.30-11.00 Coffee

Session IV. Multiscale approach to alloys thermodynamics and magnetism

Chair: C. Wolverton

11.00 – 11.30 G. Malcolm Stocks (Oak Ridge National Laboratory, USA) “First-Principles Spin-Dynamics Studies of the Magnetic Structure of Alloys and Nanostructures”
11.30 – 12.00 Balazs Gyorffy (University of Bristol, UK) “First Principles Landau Theory of Symmetry Breaking in Solids”
12.00 – 12.30 Andrej Ruban (Royal Institute of Technology, Sweden) "Magnetism and effective chemical interactions in alloys"

12.30 – 13.30 Lunch

Session V. Alloys: from the bulk towards low-dimensional and nanoscale systems

Chair: Axel van de Walle

13.30 – 14.00 Bernd Schönfeld (Department of Materials, ETH Zürich, Switzerland) ”Bulk and near-surface microstructure of alloys – diffuse scattering studies”
14.00 – 14.30 Harald Reichert (Max-Planck-Institut, Germany) “Fluctuations in binary alloys”
14.30 – 15.00 Micha Polak (Ben-Gurion University, Israel) “Extracting coordination-dependent bond-energy variations from surface-energy anisotropies for the study of alloy nanocluster surface properties”
15.00 – 15.30 Hugues Dreysse (Institut de Physique et Chimie des Matériaux de Strasbourg, France) "Equilibrium size distribution of 1D surface clusters”

15.30-16.00 Coffee

Session VIII. Nitrides and semiconductor alloys

Chair: A. Zunger

16.00 – 16.30 Sandro Scandolo (International Centre for Theoretical Physics, Italy) "Dinitrogen units in a new class of transition metal nitrides"
16.30 – 17.00 Joerg Neugebauer (Max-Planck-Institute, Germany) "Thermodynamic versus Kinetic Stabilization of Short and Long-Range Order in Nitride Based Alloys"
17.00 – 17.30 Pavel Korzhavyi (Royal Institute of Technology, Sweden) "Atomic and magnetic ordering in dilute magnetic semiconductors: effects of charge state"

18.00 - 19.00 **Poster session II**

19.00 - 20.30 Dinner

20.30 - **Poster session II**

Tuesday, June 19

Session VII. Hydrides and oxides

Chair: M. Asta

9.00 – 9.30 Chris Wolverton (Northwestern University, USA), "Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach"
9.30 – 10.00 Sergei Simak (Linköping University, Sweden) "Doped ceria from first principles"
10.00 – 10.30 Ben Burton (National Institute of Standards and Technology, USA), "The effects of chemical order and Pb-O divacancies on the ferroelectric to relaxor transition in Pb(Sc_1/2Nb_1/2)O3"

10.30-11.00 Coffee

Session VI. Alloys as structural materials

Chair: I. A. Abrikosov

11.00 – 11.30 Börje Johansson (Royal Institute of Technology, Sweden) "Stacking-fault energies in stainless steels"
11.30 – 12.00 Marcel Sluiter, (Delft University of Technology, The Netherlands) "Phase stability of carbide phases in alloyed steel from first principles"
12.00 – 12.30 Adam Kiejna (University of Wroclaw, Poland) "Effect of chromium on grain boundary cohesion in iron"

12.30-13.30 Lunch

Session IX. Surface effects

Chair: A. Ruban

13.30 – 14.00 Dario Alfe (University College London, UK), "Absolute rate of thermal desorption from first-principles simulation"
14.00 – 14.30 Matti Alatalo (Lappeenranta University of Technology, Finland) “The role of phonons and surface defects in O2 adsorption on Cu(100)”
14.30 – 15.00 Mark Asta (University of California, Davis, USA) ” Nanometer-Scale Phase Separation in Epitaxial Alloy Films”

15.00-15.30 Coffee

15.30 -17.00 Discussion and closing

List of Participants

Igor Abrikosov, Linköping University, Sweden
Graeme Ackland, University of Edinburgh, UK
Matti Alatalo, Lappeenranta University of Technology, Finland
Dario Alfe, University College London, UK
Björn Alling, Linköping University, Sweden
Ingegärd Andersson, Linköping University, Sweden
Mark Asta, UC Davis, USA
Ben Burton, National Institute of Standards and Technology, USA
Karin Carling, Karlstad University, Sweden
Stefaan Cottenier, Katholieke Universiteit, Belgium
Ralf Drautz, University of Oxford, UK
Hugues Dreysse, Universite Louis Pasteur, France
Leonid Dubrovinskii, Bayreuth, Germany
R. D. Eithiraj, Anna University, India
Marcus Ekholm, Linköping University, Sweden
Subhradip Ghosh, Indian Institute of Technology Guwahati, India
Oscar Grånäs, Dept. of Physics, Uppsala, Sweden
Ricardo Grau-Crespo, University College London, UK
Balasz Györffy, University of Bristol, UK
Thomas Hammerschmidt, University of Oxford, UK
Olle Hellman, Linköping University, Sweden
Tilmann Hickel, Max-Planck-Institut fur Eisenforschung GmbH, Germany
Qing-Miao Hu, Chinese Academy of Sciences, China
Roberto Iglesias, Paul Scherrer Institut, Switzerland
Börje Johansson, KTH, Sweden, and Sandvik Steel
Duane Johnson, UIUC, USA
Sergii Khmelevskyi, Vienna University of Technology, Austria
Adam Kiejna, Uniwersity of Wroclaw, Poland
Pavel Korzhavyi, KTH, Sweden

Francois Liot, Linköping University, Sweden
Michal Lopuszynski, University of Warsaw, Poland
Tobias Marten, Linköping University, Sweden
Philippe Maugis, CIRIMAT - ENSIACET, France
Arkady Mikhaylushkin, Linköping University, Sweden
Dane Morgan, University of Wisconsin, USA
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Pär Olsson, MMC EDF R&D, France
Micha Polak, Ben-Gurion University, Israel
Peter Puschnig, University Leoben, Austria
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Marcel Sluiter, Delft, The Netherlands
Peter Steneteg, Linköping University, Sweden
Malcolm Stocks, Oak Ridge National Laboratory, USA
Axel Van de Walle, Cal Tech, USA
Anton Van der Ven, University of Michigan, USA
Victor Vinograd, University of Frankfurt, Germany
Levente Vitos, Royal Institute of Technology, Sweden
Chris Wolverton, Northwestern University, USA
Koretaka Yuge, Kyoto University, Japan
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Alex Zunger, NREL, USA
Cecilia Århammar, KTH, Sweden