Fifth International Alloy Conference

(IAC -V)

EUROPEAN SCIENCE FOUNDATION
SETTING SCIENCE AGENDAS FOR EUROPE

EUROCORES Programme
European Collaborative Research
EuroMinScI
European Mineral Sciences Initiative

ms²e
Materials science for nanoscale surface engineering

LiLi-NFM
Linköping Linnaeus Initiative for Novel Functional Materials

Organizers: N. Dubrovinskaia, *Institute of Earth Sciences, Heidelberg, Germany;* L. Dubrovinsky *Bayerisches Geoinstitut, Bayreuth, Germany;* I. A. Abrikosov, *Linköpings University, Linköping, Sweden;* A. Gonis, *LawrenceLivermore National Laboratory, Livermore, USA,* P. E. A. Turchi, *Lawrence Livermore National Laboratory, Livermore, USA.*

Local organizing committee: Natalia Dubrovinskaia, Leonid Dubrovinsky, Igor Abrikosov and Olga Vekilova

BGI
Bayerisches Geoinstitut

LINKÖPINGS UNIVERSITET

September 11-14 2008, Ruegen, Germany

Report

Fifth International Alloy Conference (IAC-V)

11-14.09.2008, Cliff-Hotel Ruegen, Germany

Summary

The triennial International Alloy Conferences (IACs) aim at the identification and promotion of the common elements developed in the study, either experimental, phenomenological, or theoretical and computational, of materials properties across materials types, from metals to minerals. To accomplish this goal, the IAC-V brought together scientists from a wide spectrum of materials science including experiment, theory, modelling, and computation, engaged in the study of a broad range of materials properties. This conference provided a forum for presentations of state-of-the-art experimental, theoretical, and computational developments in studying, understanding, and predicting the properties of materials. It also encouraged interdisciplinary contributions, such as between the fields of condensed matter physics and earth sciences and geophysics.

Main emphasis in the talks was given to the fields of basic science, e.g., electronic structure and related properties, experimental science, e.g., assessing alloy phase diagrams, semiconductor physics, mineral science, and phenomenology. The emphasis on cross-fertilization of subject matter and the interdisciplinary character of the presentations made this meeting unique.

A number of specialized sessions covered the following topics:

Electronic structure calculations for alloys (wave functions and density functional theory for excited states, the EMTO method and applications to disordered alloys, as well as an implementation of the Non-local CPA alloy theory have been addressed);

Thermodynamics of alloys (with an emphasis on configurational thermodynamics of alloys and studies of thermodynamic properties and phase diagrams from first principles, as well as on the double defect method);

Metals and alloys at high pressure and temperature: theory and experiment (new trends in high-pressure alloys synthesis, in particular, high-pressure alloying of immiscible metals, and alloys characterisation using synchrotron radiation have been shown; new experimental and theoretical results of investigations of phase transformations and structural stability in beta-brass CuZn, FeCr and Mo under pressure have been reported);

Strongly correlated materials have been presented on example of density-functional studies of Pu-U-Zr alloys as well as investigation of the influence of two-particle correlations on electron-emission spectra thermal signatures of the volume collapse in cerium;

Alloys with special properties session gave a broad overview on metastable pseudobinary alloys of transition metal nitride thin films with resultant age hardening, on binary and multicomponent phase diagrams for titanium carbonitride, as well as on para- to ferroelastic transformations in NiTi shape memory alloys and elastic constants of Pt-Sc alloys

High-pressure and thermal properties of Fe and Fe- alloys demonstrated a strong relation between earth's and materials sciences on example of mineral physics quest to the Earth's core and theoretical investigations of structural and magnetic properties of Fe and Fe based alloys under pressure

TM oxides and compounds under high pressure session broadened the scope of presented materials due to reports on HP studies of FeMgO, FeMgSiO3, FeMg, and (Mg,Fe)O systems

Atom kinetics and electron transport in alloys was demonstrated on example of Fe-Cr, Cu-Fe, and other intermetallics ((Cu,Ni)MnSb), including nano-sized precipitates in alloys, modelling

For statistics, 43 scientists from 11 countries (Sweden, USA, Germany, Russia, United Kingdom, Czech Republic, the Netherlands, Japan, France, Austria, and Israel) took part in the scientific forum. Among them there were 13 women and 10 young scientists.

Programme

September 11, Thursday

12.00-18.00 Registration

12:30- 14:00 Lunch

17:00- 17:30 Coffee

18.00 - 18.30 Conference opening

18.30-19.30
Opening session

1. I. Abrikosov "Theoretical physics, steel and alloys" – 30 min

2. Yu. Vekilov "Electronic and Thermal properties of Quasicrystalline Alloys at Low and High Temperatures" – 30 min

19:30-21:00 Dinner

September 12, Friday

7:30- 8:30 Breakfast

8.30-10.00
Electronic structure calculations for alloys

3. T. Gonis "Wave functions and density functional theory for excited states in electronic structure calculations" -30 min

4. L. Vitos "The EMTO method and applications to disordered alloys" – 30 min

5. H. Ebert "An efficient implementation of the Non-local CPA alloy theory and its application to study magnetic and transport properties" -30 min

10.00-10.30 – Coffee

10.30 – 12.30
Thermodynamics of alloys

6. A. V. Ruban "Configurational thermodynamics of alloys from first principles" – 30 min

7. V. Vinograd "The Double Defect Method" – 30 min

8. K. Masuda-Jindo "First Principles Study of Thermodynamic Properties and Phase Diagrams of High Temperature Bcc Mo-Ta-W Alloy Systems: Inclusion of liquid phase" – 30 min

9. P. Korzhavyi “First-principles thermodynamic modeling of multicomponent alloys” – 30 min

12.30-14.00 Lunch

14-00-15.00 – **discussions and posters**

15.00 -16.30
Metals and alloys at high pressure and temperature: theory and experiment

10. N. Dubrovinskaia “High-pressure alloying” – 30 min

11. S. Pascarelli “Effects of Pressure on Magneto-Elastic Properties of Alloys” - 30 min

12. T. Mohri “First principles calculation of phase equilibria and lattice expansion of Fe-Ni system” - 30 min

16.30-17.00 – Coffee

17.00-19.00

13. O. Degtyareva “Structural transformation in beta-brass CuZn compressed to 90 GPa” – 30 min

14. V. Degtyareva “Structural stability of the sigma phase FeCr under pressure to 77 GPa” – 30 min

15. A. Mikhaylushkin “Electron Concentration and Pressure-Induced Structural Changes in Alloys InA (A = Cd, Sn)” – 30 min

16. C. Asker “First-principles solution to the problem of lattice stability in Molybdenum” – 30 min

19:30-21:00 Dinner

21.30 – **after dinner panel discussion**

September 13, Saturday

7:30- 8:30 Breakfast

8.30-10.00
Strongly correlated materials

17. A. Landa “Density-functional studies of Pu-U-Zr alloys” – 30 min

18. J. Berakdar “Influence of two-particle correlations on electron-emission spectra” -30 min

19. M. Lipp “Thermal signatures of the volume collapse (VC) in cerium” – 30 min

10.00-10.30 – coffee

10.30-12.30
Alloys with special properties

20. L. Hultman “Secondary phase transformations in metastable pseudobinary alloys of transition metal nitride thin films with resultant age hardening” – 30 min

21. D. A. Andersson “First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride” – 30 min

22. W. Schmahl “Para- to ferroelectric transformations in NiTi shape memory alloys” -30 min

23. E. I. Isaev “Elastic constants of Pt-Sc alloys” -30 min

12.30-14.00 Lunch

14-00-15.00 – **discussions and posters**

15.00-17.00
High-pressure and thermal properties of Fe and Fe alloys

24. L. Dubrovinsky “Mineral physics quest to the Earth’s core” - 30 min

25. S. I. Simak “Iron and its alloys under high pressure” - 30 min

26. L. Vocadlo “Elasticity of iron phases in the Earth's core” - 30 min

27. S. Mankovsky “Structural and magnetic properties of Fe and Fe based alloys under pressure” – 30 min

17.00-17.30 – Coffee

17.30 – 19.30
TM oxides and compounds under high pressure

28. R. Ahuja “High pressure study on FeMgO, FeMgSiO3 and FeMg systems” – 30 min

29. R. Pentcheva “Cation, charge and magnetic ordering in the Fe2O3/FeTiO3 system: Insights from correlated band theory” – 30 min

30. G. Kh. Rozenberg “Metallization of TM compounds under pressure and accompanying magnetic/electronic phenomena” – 30 min

31. Natalia Skorodumova “Theoretical study of high- to low-spin transition in (Mg,Fe)O under pressure” – 30 min

20.00- Conference dinner

September 14, Sunday

7:30- 8:30 Breakfast

8.30-10.30
Atom kinetic and electron transport in alloys

32. P. Olsson “Fe-Cr modeling” – 30 min

33. W. Püschl **“**Monte-Carlo simulation of atom kinetics in intermetallics: Correcting the jump rates” – 30 min

34. V. Vaks “Stochastic statistical theory of nucleation and growth of nano-sized precipitates in alloys with application to precipitation of copper in iron” – 30 min

35. V. Drchal “Electronic, magnetic, and transport properties of halfmetallic semi-Heusler (Cu,Ni)MnSb alloys” – 30 min

10.30-11.00 – Coffee

11.00-11.10 Conference closing

12.30 Lunch and departure

Poster presentations

1. G. M. Bhuiyan “Entropy of Mixing for AgSn liquid binary alloys”

2. L. Isaeva “Dinamical stability of the defect phase of palladium hydride: ab initio studies”

3. E. Kabliman “Ab initio calculations of formation energies of the Fe-Cr sigma-phase in magnetic state”

4. A. I. Kartsev “Stability of the face-centered-cubic phases of CoN under pressure”

5. A. Lodder “Electromigration force on a proton with a bound state”

6. S. Mankovsky “Structural and magnetic properties of Cr telluride-selenide alloys”

7. O. Narygina “Fe-Ni-C system at high pressure”

8. A. Ponomareva “Tuning of magnetic state in high-pressure synthesis of cubic phase in Fe-Si system.”

9. E. Sterer “Irreversible pressure-induced amorphization of the cation deficient perovskite La1/3NbO3”

10. K. Tarafder “Phase stability in disordered alloys: An approach via augmented space recursion based orbital peeling technique”

11. O. Vekilova “First-principles investigation of multiple hydrogen occupancy of vacancies in Pd”

12. N. Bondarenko “Lattice stability of simple metals and phase transitions at ultrahigh pressure”

13. E. Zarechnaya “New HPHT boron phase”

14. L. Pourovskii “Electronic properties of rare earth monoarsenides and rare earth iron oxyarsenides”

15. W. Wunderlich “Ab-initio calculations and experiments on CoSbTi-based Half-Heusler phases for thermoelectric applications”

Abstracts

Oral presentations

I. I. Abrikosov *“Theoretical physics, steel and alloys”*

II. Yuri Vekilov *"Electronic and Thermal properties of Quasicrystalline Alloys at Low and High Temperatures"*

III. T. Gonis *“Wave functions and density functional theory for excited states in electronic structure calculations”*

IV. L. Vitos *“The EMTO method and applications to disordered alloys”*

V. H. Ebert *"An efficient implementation of the Non-local CPA alloy theory and its application to study magnetic and transport properties"*

VI. A. V. Ruban *“Configurational thermodynamics of alloys from first principles”*

VII. V. Vinograd *"The Double Defect Method"*

VIII. K. Masuda-Jindo *“First Principles Study of Thermodynamic Properties and Phase Diagrams of High Temperature Bcc Mo-Ta-W Alloy Systems: Inclusion of liquid phase”*

IX. P. Korzhavyi *“First-principles thermodynamic modeling of multicomponent alloys”*

X. N. Dubrovinskaia *“High-pressure alloying”*

XI. S. Pascarelli *“Effects of Pressure on Magneto-Elastic Properties of Alloys*”

XII. T. Mohri *“First principles calculation of phase equilibria and lattice expansion of Fe-Ni system”*

XIII. O. Degtyareva *“Structural transformation in beta-brass CuZn compressed to 90 GPa”*

XIV. V. Degtyareva *“Structural stability of the sigma phase FeCr under pressure to 77 GPa”*

XV. A. Mikhaylushkin *“Electron Concentration and Pressure-Induced Structural Changes in Alloys InA (A = Cd, Sn)”*

XVI. C. Asker *“First-principles solution to the problem of lattice stability in Molybdenum”*

XVII. A. Landa *“Density-functional studies of Pu-U-Zr alloys”*

XVIII. J. Berakdar *“Influence of two-particle correlations on electron-emission spectra”*

XIX. M. Lipp *“Thermal signatures of the volume collapse (VC) in cerium”*

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XXI. D. A. Andersson *“First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride”*

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XXIII. E. I. Isaev *“Elastic constants of Pt-Sc alloys”*

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XXVIII. R. Ahuja *“High pressure study on FeMgO, FeMgSiO3 and FeMg systems”*

XXIX. R. Pentcheva *“Cation, charge and magnetic ordering in the Fe2O3/FeTiO3 system: Insights from correlated band theory”*

XXX. G. Kh. Rozenberg *“Metallization of TM compounds under pressure and accompanying magnetic/electronic phenomena”*

XXXI. N. Skorodumova *“Theoretical study of high- to low-spin transition in (Mg,Fe)O under pressure”*

XXXII. P. Olsson *“Fe-Cr modeling”*

XXXIII. W. Püschl *“Monte-Carlo simulation of atom kinetics in intermetallics: Correcting the jump rates”*

XXXIV. V. Vaks *“Stochastic statistical theory of nucleation and growth of nano-sized precipitates in alloys with application to precipitation of copper in iron”*

XXXV. V. Drchal *“Electronic, magnetic, and transport properties of halfmetallic semi-Heusler (Cu,Ni)MnSb alloys”*

I. Theoretical physics steel and alloys

I. A. Abrikosov[1]

[1]*Linköpings University, Campus Valla, Fysikhuset, F310, SE-581 83 Linköping, Sweden*

In the century of nanotechnology, spintronics, and graphene an apparent increase of interest towards fundamental properties of steel and other alloy systems may seem somewhat surprising. In this talk I advocate that a closer look at the problem shows its extreme complexity, and therefore the alloy physics appears to be a truly challenging task for theoretical studies.

II. Electronic and Thermal properties of Quasicrystalline Alloys at Low and High Temperatures

Yu. Vekilov[1]

[1]*State Technological University "Moscow Institute of Steel and Alloys", 4, Leninskii prospect, Moscow 119049, Russia*

The electrical conductivity, optical conductivity, thermal conductivity, heat capacity of icosahedral quasicrystalline alloys are analyzed in the framework of the multicomponent Fermi surface model. The new effects are predicted.

III. Wave functions and density functional theory for excited states in electronic structure calculations

T. Gonis[1]

[1]*Lawrence Livermore National Laboratory, PO Box 808, L-371, Livermore, CA 94551, USA*

It is shown that mixed states or ensembles of quantum N-Fermion systems characterized by a probability distribution over a set of excited states can be described by means antisymmetric wave functions. These are obtained as projections of state vectors describing pure states in a higher dimensional Hilbert space corresponding to a number of N+M, with M>0 particles onto N-particle coordinate space. These wave functions allow an extension of density functional theory to excites states in a form that is essentially identical to that of the theory's ground state formulation.

IV. The EMTO method and applications to disordered alloys

L. Vitos[1]

[1]Applied Materials Physics, Department of Materials Science and Eng., Royal Institute of Technology, SE-10044 Stockholm, Sweden
[2]Condensed Matter Theory Group, Physics Department, Uppsala University, S-75121 Uppsala, Sweden 3Research Institute for Solid State Physics and Optics, P.O.Box 49, H-1525 Budapest, Hungary

The presence of the chemical and magnetic disorder hindered any previous attempt to calculate the fundamental electronic and mechanical properties of paramagnetic Fe-based alloys from first principles theories. Our ability to reach an ab initio atomistic level in this exiting field has become possible by the recently developed Exact Muffin-Tin Orbitals (EMTO) method [1,2]. This method, in combination with the Coherent Potential Approximation has proved an accurate tool in the ab initio description of the concentrated random alloys [3,4]. During the last seven years, using the EMTO method, we presented an insight to the electronic and magnetic structure, as well as structural, micro-mechanical and surface properties of simple and transition metal alloys (e.g., Al-based alloys, Hume-Rothery alloys, Pd-Ag) [4-14], Fe-Cr alloys [15-17], geomaterials (e.g., MgCaSiO3, Fe-Si, Fe-Mg, Fe-Ni) [18-23], and austenitic stainless steels [4,24-27]. In my talk, I will present the main characteristics of the EMTO method and demonstrate it through a few applications.

[1] O. K. Andersen, O. Jepsen, and G. Krier, in Lectures on Methods of Electronic Structure Calculations, edited by V. Kumar, O. K. Andersen, and A. Mookerjee, World Scientific Publishing Co., Singapore, pp. 63-124 (1994).
[2] Vitos, L. Phys. Rev. B 64, 014107 (2001).
[3] Vitos, L., Abrikosov, I. A., and Johansson, B. Phys. Rev. Lett. 87, 156401(4) (2001).
[4] L. Vitos, Computational Quantum Mechanics for Materials Engineers: The EMTO Method and Applications (Springer-Verlag, London, 2007).
[5] Magyari-Köpe, B., Grimvall, G., and Vitos, L. Phys. Rev. B 66, 064210 (2002).
[6] Magyari-Köpe, B., Vitos, L, and Grimvall, G. Phys. Rev. B 70, 052102 (2004).
[7] Taga, A., Vitos, L., Johansson, B., and Grimvall, G. Phys. Rev. B 71, 014201 (2005).
[8] Ropo, M., Kokko, K., Vitos, L., and Kollar, J. Phys. Rev. B 71, 045411 (2005).
[9] Ropo, M., Kokko, K., Vitos, L., Kollar, J., Johansson, B. Surf. Sci. 600, 904 (2006).
[10] Zander, J., Sandström, R., Vitos, L. Comp. Mater. Sci. 41, 86-95 (2007).
[11] Music, D., Takahashi, T., Vitos, L., Asker, C., Abrikosov, I. A., Schneider, M. J. Applied Physics Letters 91, 191904(3) (2007).
[12] Vitos, L., Ropo, M., Kokko, K., Punkkinen, M. P. J., Kollar, J., Johansson, B. Phys. Rev. B 77, 121401(R) (2008).
[13] Hu. Q. M., Kadas, K., Hogmark, S., Yang, R., Johansson, B., Vitos, L. Applied Physics Letters 91, 121918 (2007).
[14] Huang, L. Vitos, L., Kwon, S. K., Johansson, B., and Ahuja, R. Phys. Rev. B 73, 104203 (2006).
[15] Olsson, P., Abrikosov, I. A., Vitos, L., and Wallenius, J. J. Nuclear Materials 321, 84-90 (2003).
[16] Kissavos, A. E., Simak, A. E., Olsson, P., Vitos, L., and Abrikosov, I. A. Comp. Mat. Sci. 35, 1-5 (2006).
[17] Ropo, M., Kokko, K., Punkkinen, M. P. J., Hogmark, S., Kollar, J., Johansson, B., and Vitos, L. Phys. Rev. B 76, 220401(R) (2007).
[18] Dubrovinsky, L., et al. Nature 422, 58-61 (2003).
[19] Vitos, L., Magyari-Köpe, B., Ahuja, R., Kollar, J., Grimvall, G., and Johansson, B. Physics of the Earth and Planetary Interiors 156, 108-116 (2006).
[20] Koci, L. Vitos, L, and Ahuja, R. Physics of the Earth and Planetary Interiors 164, 177 (2007).
[21] Dubrovinsky, L., et al. Science 316, 1880 (2007).
[22] Dubrovinskaia, N., et al. Phys. Rev. Lett. 95, 245502 (2005).
[23] Kadas, K., Vitos, L., Ahuja, R. Earth and Planetary Science Letters, accepted (2008). [24] Vitos, L., Korzhavyi, P. A., and Johansson, B. Nature Materials 2, 25-28 (2003).
[25] Vitos, L., Korzhavyi, P. A., and Johansson, B. Phys. Rev. Lett. 88, 155501(4) (2002). [26] Vitos, L., Korzhavyi, P. A., and Johansson, B. Phys. Rev. Lett. 96, 117210 (2005).
[27] Vitos, L., Nilsson, J.-O., and Johansson, B. Acta Materialia 54, 3821-3826 (2006).

V. An efficient implementation of the Non-local CPA alloy theory and its application to study magnetic and transport properties

H. Ebert[1], D. Koedderitzsch[1], S. Lowitzer[1], J. Staunton[2], P. Tulip[2]

1University of Munich, Department of Chemistry and Biochemistry, Germany
2 University of Warwick, Great Britain

The Coherent Potential Approximation (CPA) is a widely used scheme to describe the electronic properties of disordered alloys. In spite of its restrictive assumption of a random occupation of lattice sites it is rather successful in most situations. Recently, an extension to the CPA has been introduced - called non-local CPA (NL-CPA) - that removes this restriction and allows accordingly to deal with the influence of atomic short range order (SRO). We present an efficient implementation of the NL-CPA in combination with the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) band-structure method. As an application of the NL-CPA-SPR-KKR we present results of investigations on various magnetic properties (spin and orbital magnetic moments, hyperfine fields) for a number of transition metal alloys. Special emphasis is laid on the fluctuations around the alloy configurational average. As a second application, we present a combination of the NL-CPA with the Kubo-Greenwood formalism used to deal with the residual resistivity of alloys. It is demonstrated for different types of transition metal alloys that the combined approach indeed allows to deal with the impact of SRO on the residual resistivity.

VI. Configurational thermodynamics of alloys from first principles

A. V. Ruban[1]

[1]CAMP, Physics Department, Technical University of Denmark, Bldg. 307, Lyngby 2800 Denmark

Effective cluster interactions of an Ising-type Hamiltonian provide the only efficient way for solving configurational thermodynamics problems in alloys. This talk gives a short overview of both the general properties of effective cluster interactions and first principles methods of their determination.

VII. The Double Defect Method

V. Vinograd[1]

1Swedish Museum of Natural History, Frescativagen 40, Stockholm 10405 Sweden

Complete set of composition-dependent pairwise effective cluster interactions (ECIs) of a binary (A,B)R solid solution is determined from the excess enthalpies of supercell structures prepared from the end-members AR and BR by inserting double defects of BB- and AA-type, respectively, at all distances permitted by the supercell size. The excess enthalpy of any A/B configuration in the supercell is written as the sum of the pair ECIs multiplied by corresponding numbers of AB pairs. The temperature-dependent enthalpy of mixing is simulated with the Monte Carlo method, while the Gibbs free energy of mixing is obtained from the enthalpies by thermodynamic integration. Since the structures with the double defects are generated using a fully deterministic principle, and since the number of such structures is limited, calculations with ab initio methods in large supercells become feasible. Solid solutions in CaCO3-MgCO3, TiO2-SiO2, MgSiO3-Al2O3 and SiC-AlN systems are considered.

VII. First Principles Study of Thermodynamic Properties and Phase Diagrams of High Temperature Bcc Mo-Ta-W Alloy Systems: Inclusion of liquid phase

K. Masuda-Jindo[1], Vu Van Hung [2], and P.E.A Turchi[3]

[1]*Department of Materials Science and Engineering, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama 226-8503, Japan*
[2] *Department of Physics, Hanoi National Pedagogic University, km8 Hanoi-Sontay Highway, Hanoi, Vietnam*
[3] *Lowewnce Livermore National laboratory, PO Box 808, L-353 LLNL, Lovermore CA 94551 U.S.A.*

The thermodynamic quantities of metals and alloys are studied using the moment method in the quantum statistical mechanics [1-4], going beyond the quasi-harmonic approximations. In addition to the thermodynamic quantities like thermal lattice expansions, specific heats, Grüneisen constants, elastic moduli of solid phases, we also calculate the free energies and thermodynamic quantities of liquid phases. The first principles calculations of alloy phase diagrams by combined statistical moment and cluster variation methods are presented. Including the power moments of the atomic displacements up to the fourth order, the free energies of alloy systems are derived explicitly in closed analytic forms. The configulational entropy term is taken into account by coupling the moment expansion scheme with the cluster variation method (CVM). The free energies of liquid phases are evaluated by using the Gibbs-Bogoliubov variational theory, starting from the reference state given by the modified hard-sphere model. The internal energies of the alloys are evaluated by using the first principles TB-LMTO-CPA-GPM method [5]. The applications of the present scheme are given for the high temperature binary Ta-W and Mo-Ta alloys as well as the ternary Mo-Ta-W alloys. The calculated thermodynamic quantities and equilibrium phase diagrams, including the liquidus and solidus lines, by the first principles statistical moment and cluster variation methods are in good agreement with the available experimental results.

[1] Vu Van Hung, K. Masuda-Jindo and P.T.M. Hanh, J. Phys.: Condens Matter 18, (2006) 283.
[2] Vu Van Hung, J. Lee and K. Masuda-Jindo, J. Phys. Chem. Sol., 67, (2006) 682.
[3] K. Masuda-Jindo, Vu Van Hung and P.E.A. Turchi, Solid State Phenomenna 138, (2008) pp 209.
[4] K. Masuda-Jindo, Vu Van Hung, N. T. Hoa and P.E.A. Turch, J Alloy & Compounds 452, (2008) 127.
[5] P. E. A. Turchi, V. Drchal, J. Kudmocský, C. Colinet, Larry Kaufman and Zi-Kui Liu, Phys. Rev. B71, (2005) 094206.

IX. First-principles thermodynamic modeling of multicomponent alloys

P. Korzhavyi[1]

[1]*Department of Materials Science and Engineering, Royal Institute of Technology (KTH), Brinellvägen 23, 100 44 Stockholm, Sweden*

Practical aspects of modeling multicomponent alloys using first-principles calculations will be discussed. The discussion will be based on the results of our recent studies of high-alloy steels and refractory compounds.

X. High Pressure Alloying

N. Dubrovinskaia[1]

[1]*Department of Mineralphysics, Institute of Earth Sciences, University of Heidelberg, Im Neuenheimer Feld 236, D-69120 Heidelberg, Germany*

Over the past decade, high pressure experimental technique and modern physical methods of probing of materials properties have evolved so much that the high pressure research has become a scientific direction of a broad interdisciplinary importance. High-pressure studies provide crucial information for many scientific and industrial applications, because pressure-induced volume changes can produce structural, electronic, magnetic, and other phase transitions, initiate chemical reactions, and many other phenomena.

Alloying is one of the most efficient ways of improving materials' performance. The iron-based alloys (steels) are at the heart of the modern industry. Magnesium-based alloys (first of all with aluminum, zinc, and lead) are rapidly making their way into different technological applications. At the same time, iron-magnesium alloys have not been synthesized yet, because Fe and Mg are almost immiscible at ambient pressure due to a very large size mismatch between the alloy components. However, the compressibility of Mg is much higher than that of Fe, and therefore the difference in atomic sizes between elements decreases dramatically with pressure.

We will address technical aspects and a generality of the concept of possible high-pressure alloying between immiscible elements on example of iron group elements (Fe, Co, Ni) and magnesium. We will also show other perspectives for formation of solid solutions under pressure on example of boron doped diamonds.

XI. Effects of Pressure on Magneto-Elastic Properties of Alloys

S. Pascarelli[1]

[1]*CEA/Le Ripault, DAM/DMAT, BP16, F-37160 Mont France*

Recent developments in the field of synchrotron radiation based methods have enabled the measurement of femtometer atomic displacements [1] using X-ray Absorption Spectroscopy. In principle any reproducible subtle distortion of the local structure induced by an external perturbation can now be investigated and quantified at ambient as well at high pressure. Phenomena such as magnetostriction, electrostriction, piezoelectric or magnetic effects, elastic compliance or thermal expansion may be investigated from an atomic point of view, so that we can understand which atomic movements are responsible for the macroscopic effect that we observe.

Up to now, experimental input relied essentially on macroscopic quantities where the important atomic information is averaged out over different chemical bonds, defects, etc. Being able to be not only “local” but also “chemical selective” opens an enormous potential for the study of complex and disordered systems.

We have very recently applied this new method to address the complex problems of magnetoelastic coupling and magnetostriction at the atomic level [2]. One of the first problems we addressed is the investigation of local atomic displacements induced by anisotropic magnetostriction in FeCo and how these are affected by a modification of the volume of the unit cell. Here magnetoelastic coupling is found to favor enhancement of atomic displacements with decreasing volume, contrary to expectations based only on the commonly accepted “stiffening” of bonds with compression. State-of-the-art ab-initio electronic structure calculations of the evolution of magnetocrystalline anisotropy energy with tetragonal strain in FeCo are found capable of predicting correctly even such tiny effects, where the energies in play are of the order of the micro-eV. This kind of information, obtained through the combination of experiment and theory, is fundamental to be able to guide the search for materials with improved properties.

[1] “The measurement of tiny displacements using X-ray absorption spectroscopy” R. Pettifer, O. Mathon, S. Pascarelli, M. Cooke and M. Gibbs, Nature 435, 78 (2005)

[2] "Effect of Pressure on Magnetoelastic Coupling in 3*d* Metal Alloys Studied with X-Ray Absorption Spectroscopy"S. Pascarelli, M. Ruffoni, A. Trapananti, O. Mathon, G. Aquilanti, S. Ostanin, J. B. Staunton, and R. F. Pettifer, Physical Review Letters 99, 237204 (2007)

XII. First principles calculation of phase equilibria and lattice expansion of Fe-Ni system

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By combining FLAPW electronic structure total energy calculations with Cluster Variation Method, first-principles calculation of phase equilibria for Fe-Ni system has been attempted. Although FeNi-L10 ordered phase is missing in the conventional phase diagaram, our first-principles calculation indicates that FeNi is stabilized below 500K. Coefficient of thermal expansion is calculated for an entire composition range and non-monotonic behaviour is found above 50%Fe including invar composition.

XIII. Structural transformation in beta-brass CuZn compressed to 90 GPa

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Cu–Zn is a classic example of an alloy system displaying a sequence of phases along an alloy composition, called Hume-Rothery phases. The crystal structure of these phases is determined by electron concentration (that is the number of valence electrons per atom), and the lowering of the electronic energy is considered the key factor for the structure stabilization. And because high pressure enhances this stabilization factor, it would be interesting to look at the structural stability of the Hume-Rothery phases on compression. In our resent high-pressure studies [1] we looked at the alfa-, beta- and gamma-phases of Cu-Zn with the fcc, bcc and complex cubic structures, respectively, in the pressure range up to 50 GPa. We found that the alfa- and beta-phases show a structural distortion at 17 and 37 GPa, respectively, while the gamma-phase remained stable up to the maximum pressure of this study. In our present study we look in detail at the structural distortion of the beta-phase of CuZn in the pressure range up to 90 GPa. We used the synchrotron x-ray diffraction technique at the HPCAT station of the Advance Photon Source (Argonne National Lab) and diamond anvil cells to generate pressure. In the diffraction patterns above 40 GPa we observed splitting of the bcc reflections, as well as appearance of weak superstructure reflections. Splitting of the main reflections is explained by a trigonal distortion of bcc, while the additional reflections are due to a positional modulation along the trigonal axis. We analyze the structural distortion of the bcc phase CuZn by looking at the configuration of the Brillouin zone of the bcc and the trigonal structures and their interaction with the Fermi surface using the program BRIZ [2]. The number of planes in the Brillouin zone increases, zone filling with electronic states increases from 75% (bcc) to 81% (trigonal structure). This brings more of the lower-energy electrons in states of higher density and the overall electronic energy is expected to be reduced. These factors indicate an enhancement of the Hume-Rothery mechanism under pressure.

[1] V.F. Degtyareva et al, J. Phys. Condens. Matter 17, 7955 (2005)
[2] V.F. Degtyareva and I.S. Smirnova, Z. Kristallogr. 222 718–721 (2007)

XIV. Structural stability of the sigma phase FeCr under pressure to 77 GPa

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Fe–Cr alloy system contains an intermediate phase of the equiatomic composition called the sigma phase. The crystal structure of the sigma phase is tetragonal with 30 atoms in the unit sell, space group P42/mnm, lattice parameters a=8.7995 Å, c=4.5442 Å, c/a=0.516, Pearson symbol tP30 [1], whereas pure elements Fe and Cr both crystallize in the body-centered cubic (bcc) structure. The aim of this work was to investigate the stability of the FeCr sigma phase at high pressure. Diffraction studies of the FeCr sample with the sigma phase were performed using diamond anvil cell, image plate detector and synchrotron radiation at the Advanced Photon Source (Argonne National Lab). The highest pressure achieved in this study was 77 GPa. The sigma phase was found to be stable in this pressure range. The equation of state for the tetragonal structure was found to have the values of bulk modulus Ko=217(5) GPa and Ko'=5.8(2). Interestingly, the compressibility of the FeCr sigma phase is lower than that of the constituent elements. Structural stability of the sigma phase under pressure found in the present study supports the suggestion that electronic energy is one of the main factors responsible for the existence of this complex, low-symmetry structure. The stability of the sigma phase can be related to the Hume-Rothery effects based on the Fermi surface – Brillouin zone interactions. [2]. Partial support from RFBR under grant 07-02-00901 is acknowledged.

[1] G. Bergman and D. P. Shoemaker, Acta Crystallogr. 7, 857 (1954).
[2] V. F. Degtyareva and I. S. Smirnova, Z Kristallogr. 222, 718 (2007).

XV. Electron Concentration and Pressure-Induced Structural Changes in Alloys InA (A = Cd, Sn)

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Electron concentration and pressure induced structural transitions in solid solutions In1-xCdx ($0 < x < 0.1$) and In1-xSnx ($0 < x < 0.2$) have been investigated by means of first principles calculations. At ambient pressure the structural sequence face-centred cubic (fcc) body-centred tetragonal ($c/a > \sqrt{2}$ (bct-I); body-centred tetragonal ($c/a < \sqrt{2}$) (bct-II) is realized with increasing of valence electron concentration (VEC). High pressure has the same effect as the increase of electron concentration shifting the occurrence of the structural transitions to lower valence electron concentration. The driving force behind the peculiar structural sequence is an enhancement of s-p hybridization with increasing VEC.

XVI. First-principles solution to the problem of lattice stability in Molybdenum

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The concept of lattice stability is defined as the difference in Gibbs energy between different crystallographic structures. For the transition metals in the middle of the series, there are large disagreements between the lattice stability obtained by the thermochemical (CALPHAD) approach based on the analysis of experimental data, or by ab-initio electronic structure calculations. We have investigated this problem for the case of the lattice stability in Mo. Earlier, zero temperature calculations indicated that the configurational energy difference between bcc and fcc Mo is around 0.40 eV/atom [1], while the CALPHAD results is estimated to be 0.18 eV/atom [2, 3] for T=3000K. The fcc structure of Mo is known to be dynamically unstable at ambient conditions, that is, it has complex phonon frequencies in some parts of the phonon spectrum. We show that this structure can be stabilized at high temperatures. By including temperature through ab-initio molecular dynamics simulations for the bcc and fcc structures at high temperature, we have found that the configurational energy difference reduces to 0.19 eV. While the stabilization is partly due to a change of occupation of states near the Fermi level because of high temperature, the main effect comes from the modification of the canonical band structure due to anharmonic thermal motion at high temperature.

[1] A.T. Dinsdale. Calphad, 15:317, 1991.
[2] H. L. Skriver. Phys. Rev. B, 31:1909, 1985
[3] Y. Wang et al. Calphad, 28:79, 2004.

XVII. Density-functional studies of Pu-U-Zr alloys

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Zr-based actinide alloys, particularly U-Zr and U-Pu-Zr, proved to be very promising fuels for liquid metal fast breeder reactors because of their advantages in view of superior performance, reactor safety, and fuel cycle economies. In spite of renewed interest in Zr-based actinide alloys from a practical view point, very little has been done to understand fundamental aspects of phase equilibria in these systems. First, we employ first-principles methods to study the ground-state properties of gamma (bcc) and delta UZr2 (C32) phases of the U-Zr system. The binodal decomposition curve for bcc-based U-Zr solid solutions is derived from Ising-type Monte Carlo simulations incorporating effective interatomic interactions obtained from the screened general perturbation and KKR-ASA-CPA methods. The EMTO-CPA method is applied to study properties of the 'open' delta phase. Results of ab initio calculations are compared with experimental data and CALPHAD assessment. We also explore the idea of stabilization of the UZr2 phase against the alpha-Zr (hcp) structure due to increase of Zr d-band occupancy by the addition of U to Zr. Analogy with stabilization of the omega phase in Zr under compression is made. Finally, we present some ab initio results of the electronic structure calculations for Pu-Zr and Pu-U alloys.

XVIII. Influence of two-particle correlations on electron-emission spectra

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Formal analysis based on the many-body perturbation theory reveals the conditions under which short-range two-particle correlation in condensed matter can be mapped by means of the coincident two-particle emission. The spectra of the two-electrons can be related to the two-particle spectral density. Numerical results for this quantity are obtained from the dynamical mean field theory (DMFT) for the Hubbard model and are analyzed in view of existing experiments.

XIX. Thermal signatures of the volume collapse (VC) in cerium

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Despite extensive experimental and theoretical efforts, much of the available information about the phase diagram of cerium and especially its large VC appears incomplete or controversial. Results are easily affected by sample treatment or have been obtained several decades ago. Only a few investigations exist at higher temperature near the critical point of the VC. However, precise knowledge of the equation of state (EOS) especially at temperatures higher than the critical point - whose location itself is under debate - would benefit modern theoretical calculations expecting the cause of the VC to be of purely electronic origin. In that case some remnant of the VC might persist as a softness of the EOS, possibly extending into the liquid phase. High precision P-V isotherms obtained at a 3rd generation synchrotron will be shown and discussed with regard to whether modern p-V data can help constrain theoretical advances and whether modern theoretical tools can successfully – i.e. quantitatively - model those data. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

XX. Secondary phase transformations in metastable pseudobinary alloys of transition metal nitride thin films with resultant age hardening

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The concept of age hardening is introduced for supersaturated cubic-phase transition metal nitride alloy systems. Secondary phase transformation including spinodal decomposition of TiAlN into coherent cubic-phase nm-size domains of TiN and AlN is thus demonstrated by experiments coupled with ab initio calculations. The as-formed domains hinder dislocation glide in films annealed to temperatures corresponding to cutting tool operations.

XXI. First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride

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We have used a combined first principles and Calphad approach to model phase diagrams in the titanium-carbon-nitrogen system and we have paid particular attention to the vacancy-induced ordering of the substoichiometric carbonitride phase, TiC_xN_y ($x+y \leq 1$). Results from earlier Monte Carlo simulations of the low-temperature binary phase diagrams were used in order to construct sublattice models for TiC_xN_y within the compound energy formalism (CEF) that are capable of describing both the low-temperature ordered and the high-temperature disordered state. We parameterize these models using first-principles calculations and then we demonstrate how they can be merged with thermodynamic descriptions of the remaining Ti-C-N phases that are derived within the Calphad method by fitting model parameters to experimental data.

XXII. Para- to ferroelectric transformations in NiTi shape memory alloys

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The NiTi alloy system is most promising for shape memory and superelastic applications. Both effects are related to a martensitic phase transition, i.e. a diffusionless 1st order paraelastic-ferroelastic phase transition. The shape memory effect occurs in conditions where the ferroelastic phase is stable. An applied stress will move the domain walls between ferroelastic twins. Accordingly, favourably oriented ferroelastic domains will grow at the expense of others and this results in a macroscopic shape change. The obtained shape change (domain configuration) remains when the stress is released. Heating to the paraelastic phase and zero-field cooling will restore a random domain configuration, restoring the original shape. Superelasticity occurs in conditions where the paraelastic phase is stable. Application of a stress field exceeding a critical strength will transform the paraelastic phase to the ferroelastic phase with an stress-adapted domain configuration. This is associated by a shape change. When stress is released the material transforms back to the paraelastic phase recovering the original shape. The transition temperature varies drops dramatically from 325 K to 200 K with Ni content between Ni50Ti50 and Ni51Ti49, and this can be used to tune the materials behaviour at application temperatures. Matters are complicated by the fact that there is a second ferroelastic NiTi phase of trigonal symmetry, and there are semicoherent nanoscale precipitates of a rhombohedral Ni4Ti3 phase which improve the superelastic engineering properties. In situ studies of NiTi alloys with synchrotron and neutron techniques reveal phase stabilities and domain preferred orientation under applied load. The structural order parameter of the monoclinic phase is still enigmatic and it is an open question which effects, elastic and/or electronic, control the phase stability relations.

XXIII. Elastic constants of Pt-Sc alloys

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The exact muffn-tin orbitals (EMTO) technique, in conjunction with the coherent potential approximation (CPA), has been used to calculate the elastic constants and evaluate related mechanical properties of substitutionally disordered fcc Pt-Sc alloys, calculated as a function of composition and those of L12 -ordered intermetallic compound Pt3 Sc. Based on analysis of these properties we have shown that Pt-Sc alloys are quite ductile and, at the same time, possess high strength compared to conventional Ni-Al superalloys that makes Pt-Sc alloys high potentially superalloys. This work was supported by The Russian Foundation for Basic Researches (grant 07-02-01266) and The Swedish Foundation for Strategic Research (SSF, programme INALLOY).

XXIV. Mineral Physics Quest to the Earth's Core

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Understanding the Earth's core requires multidisciplinary efforts to untangle its complex nature using seismic observations, geodynamic modelings, geochemical measurements, and mineral physics results. These resilient efforts of deep-Earth scientists have recently unveiled a number of unusual and enigmatic phenomena of the core. Among them are the inner core anisotropy, differential rotation between the inner core and the rest of the Earth, fine–scale seismic heterogeneity, as well as possible existence of the preferred-orientated hexagonal closest-packed (*hcp*) and/or body-centered cubic (*bcc*) iron-nickel-light element alloys in the inner core.

We summarize some new results about the nature of the core from recent mineral physics experiments and theory, highlighting new ideas about the core's composition and crystal structure, melting curve, and sound velocities and anisotropy of candidate iron alloys at extreme pressure-temperature conditions. Recent advances and future challenges in the mineral physics quest to the core are emphasized to stimulate frontier multidisciplinary efforts in understanding the Earth's core.

XXV. Iron and its alloys under high pressure

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Cosmochemical, geochemical, and geophysical studies indicate that Earth's core contains iron with substantial (5 to 15%) amounts of nickel. We address structural properties of pure and nickel-doped iron from both first-principles theory and experiment. In particular we show that the face-centered cubic (fcc) phase may become as stable as the hexagonal close-packed (hcp) phase at pressures around 300-360 GPa and temperatures around 5000-6000 K, corresponding to the Earth's core conditions [1]. Our temperature-quenched experiments indicate that the face-centered cubic (fcc) phase of pure iron can exist in the pressure-temperature region above 160 GPa and 3700 K. Further, we show that at pressures above 225 GPa and temperatures over 3400 K, $Fe_{0.9}Ni_{0.1}$ alloy adopts the body-centered cubic (bcc) structure [2].

[1] A.S. Mikhaylushkin, S.I. Simak, L.S. Dubrovinsky, N. Dubrovinskaia, B. Johansson, and I. A. Abrikosov, Phys. Rev. Lett. 99, 165505 (2007)

[2] L. S. Dubrovinsky et al., Science B 316, 1880 (2007).

XXVI. The phase stability and elastic properties of iron and iron alloys at inner core conditions.

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There are many unresolved problems concerning our understanding of the Earth's inner core; even fundamental properties, such as its internal structure and exact composition, are poorly known. Although it is well established that the inner core is made of iron with some alloying element(s), the structural state of the iron and the nature of the light element(s) involved remain controversial. Furthermore, seismically observed P-waves show the inner core to be anisotropic and layered, but the origins of this are not understood; seismically observed S-waves add to the complexity as they have unexpectedly low velocities. Seismic interpretation is hampered by the lack of knowledge of the physical properties of core phases at core conditions. Moreover, the resolution of seismic data are hampered by the need to de-convolve inner core observations from seismic structure elsewhere in the Earth; this is particularly relevant in the case of shear waves where detection is far from straightforward. If we had sufficiently well constrained seismological data, together with accurate high-pressure, high-temperature elastic properties of the candidate materials, we could, in principle, fully determine the structure and composition of the inner core - an essential prerequisite to understanding its evolution. Unfortunately, the extreme conditions of pressure and temperature required make results from laboratory experiments unavoidably inconclusive. However, computer simulations of materials at inner core conditions are now achievable. *Ab initio* molecular dynamics simulations have been used to determine the stable phase(s) of iron in the Earth's core and to calculate the elasticity of iron and iron alloys at core conditions. The calculated shear wave velocities are significantly higher than those inferred from seismology. If the seismological observations are robust, then a possible explanation for this discrepancy is if the inner core contains a significant amount of melt. The observed anisotropy can only be explained by almost total alignment of crystals present.

XXVII. Structural and magnetic properties of Fe and Fe based alloys under pressure

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The investigations of structural and magnetic properties of Fe and Fe-based alloys (Fe-Pt, Fe-Ni) under pressure have been performed on the basis of electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) band structure method. Analysis of structure stability is based on the total energy and phonon spectra calculations. The magnetic structure and critical temperatures were obtained within the Monte Carlo simulations based on Heisenberg model with the exchange coupling parameters calculated from first principles.\\

The pressure dependent X-ray absorption (XAS) and X-ray magnetic circular dichroism (XMCD) spectra were calculated and compared with those obtained experimentally. Both results are in a good agreement with each other. In the case of pure Fe, an analysis of experimental and theoretical results gave us a possibility to explain the differences in behaviours of magnetic and structural signals under pressure observed experimentally. The role of magnetism in stabilisation of bcc structure as well as in structural bcc to hcp transition was also analysed.

XXVIII. High pressure study on FeMgO, FeMgSiO3 and FeMg systems

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We investigated structural and electronic behaviours of $MgSiO_3$ crystals dissolved with Fe under pressure up to that in the Earth's lower mantle using the first-principles theory. Local relaxation occurs around the Fe ions. The Fe-dissolving $MgSiO_3$ crystals have phase transform from the orthorhombic perovskite (OPv) structure into the orthorhombic post-perovskite (OPPv) phase and the transition pressure decreasing with increasing Fe concentration. In the configurations of one Si-Mg pair replaced by two Fe atoms, the F^{2+}-Fe^{4+} pairs cause rather strong local distortion in the OPv structure that the transition pressure strongly decreases. Electronic transitions occur in the pressure range of about 70 to 90 GPa for an $(Mg,Fe)(Si,Fe)O_3$ OPv crystal, in which the moment of the Fe^{4+} ion decreases gradually to zero at which the magnetic moment of the Fe^{2+} ion becomes zero. That electronic transition provides the possible mechanism to understand recent experiments. Further, we have also study FeMgO and FeMg under very high pressure.

XXIX. Cation, charge and magnetic ordering in the Fe_2O_3/FeTiO Fe_2O_3/ system: Insights from correlated band theory

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Charge mismatch at complex oxide interfaces can give rise to properties and functionality entirely different from the parent compounds. For example nanoscale lamellar exsolutions between the canted antiferromagnet haematite and the room temperature (RT) paramagnet ilmenite show unique magnetic properties. To explain the origin of magnetism in the Fe_2O_3-$FeTiO_3$ system we have performed density functional theory calculations systematically varying the concentration, distribution and charge state of Ti (Fe) incorporated in a α-Fe_2O_3 ($FeTiO_3$) host. We use the all-electron full-potential linearized augmented plane wave method in the WIEN2k implementation. Including electronic correlation within the LDA+U approach is found to be decisive to obtain the correct magnetic ground state and band gap of the end members, $Fe^{3+}{}_2O_3$ and $Fe^{2+}Ti^{4+}O_3$.

The phase diagram of the stability with respect to the end members for more than 30 different configurations reveals a clear preference to form layered arrangements as opposed to solid solutions. We find that the charge mismatch at the interface between Fe_2O_3 and $FeTiO_3$ is accommodated through Ti^{4+} and a disproportionation in the Fe contact layer into Fe^{2+}, Fe^{3+}. This leads to uncompensated moments in the contact layer and gives first theoretical evidence for the lamellar magnetism hypothesis [1]. This interface magnetism is associated with impurity levels in the band gap showing half-metallic behaviour [2] and making Fe_2O_3/$FeTiO_3$ heterostructures prospective materials for spintronics applications.

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[1] P. Robinson, et al., Nature 418, 517 (2002).
[2] R. Pentcheva, H. Sadat Nabi, Phys. Rev. B, 77, 172405 (2008)

XXX. Metallization of TM compounds under pressure and accompanying magnetic/electronic phenomena

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The main purpose of this lecture is to address the issue of magnetic/electronic phenomena and related crystallographic transitions in strongly correlated TM compounds, particularly Fe-containing compounds, in a regime of very high static density. We'll focus on the following examples:

(i) Sluggish structural phase transitions in antiferromagnetic insulators FeI_2 and $FeCl_2$ attributed to the onset of a Mott transition (MT). These studies show a precursor intermediate pressure phase formation preceding the MT and allow establishing features of the structural transformation specifically attributed to the MT for different types of the electronic transitions (Mott-Hubbard and Charge-Transfer).

(ii) Volume dependence of the orbital term of the moment in FeI_2 and $FeCl_2$ results in its eventual collapse under pressure. For these compounds significant lattice distortion is observed attributed to the quenching of the orbital term, and this transformation further culminates into a Mott transition.

(iii) High-spin (HS) to low-spin (LS) transition, a result of Hund's rule breakdown at very high density. Such a transition will be accompanied by a significant reduction of the TM ionic radii and therefore a volume decrease or even a structural transition.

(iv) PI intervalence charge transfer in the layered antiferromagnetic $Cu^{+1}Fe^{3+}O_2$ delafossite as a result of increase in band overlap. This process results in part of the Fe^{3+} converting into Fe^{2+} concurrent with $Cu^{1+} \rightarrow Cu^{2+}$ partial transition with the creation of the new Cu^{2+} - Fe^{2+} magnetic sublattice. XRD studies have shown a structural phase transition leading to the breakage of the dumb-bell like O-Cu-O bonds which results in the stabilization of the antifferomagnetic order and culminating into valence transformation.

(v) PI reversible charge reorganization of the octahedral (*B*) and tetrahedral (*A*) sites in magnetite resulting into *inverse*- to *normal-spinel* transition. The configuration transformation is reflected by the increase of the tetrahedral volume as a result of the $(Fe^{3+}\rightarrow Fe^{2})_A$ transition, and a decrease of the octahedral volume as result of the $(Fe^{2+},Fe^{3+})_B\rightarrow(Fe^{3+}+ Fe^{3+})_B$ transition.

XXXI. Theoretical study of high- to low-spin transition in (Mg,Fe)O under pressure

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Correct interpretation of the seismic structure of Earth in terms of materials composing our planet requires the detailed knowledge of the physical properties of various metal oxides. (Mg,Fe)O is one of the host materials of the lower mantle. Under pressure this material exhibits high- to low-spin transition that effects its elastic, electrical and optical properties. Here we report the results of our ab initio study of this transition and discuss the electronic structure and elastic properties of the high- and low-spin phases.

XXII. Modelling of FeCr alloys for nuclear applications

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FeCr alloys have garnered renewed interest during the last years, due to the foreseen use of Ferritic/Martensitic steels of high Cr content in future nuclear installations. Especially interesting as a model system is the binary FeCr since the Cr content has a major influence on the evolution of the mechanical properties in irradiated Ferritic/Martensitic alloys. Experimentally, these alloys have been studied for over 40 years, but for a long time the understanding of many observed effects was lacking. Already 20 years ago calculations appeared that indicated the relevance of the concentration, in terms of the inversion of short range ordering around 10% Cr. However, these studies were not extensively followed up until recently. Here we will discuss the latest developments in the multi-scale modeling efforts, based on density functional theory, of thermodynamics and defect properties in FeCr alloys and how the understanding of the microscopic origins of macroscopic effects is evolving.

XXXIII. Monte-Carlo simulation of atom kinetics in intermetallics: Correcting the jump rates.

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The favorable properties of intermetallics such as mechanical strength, corrosion resistance and magneto-crystalline anisotropy are strongly dependent on long-range order. The temperature dependence of its equilibrium value, the rate at which it is attained, and the stability of non-equilibrium states thus are important parameters of materials behavior. For this reason we need to understand in detail the kinetics of order. Monte-Carlo (MC) simulation offers itself as a natural method of re-enacting the statistical effect of many atom jumps. The method has a more mathematical aspect concerning the way the single atom jump is treated as a Markov process (Metropolis/Glauber versus Residence time algorithms), and a more physical aspect concerning the modeling of the atom jump itself and the rate at which it takes place. Although in many cases a direct-exchange mechanism may be used as an approximate kinetic model, the real physical situation in the materials considered here corresponds to a vacancy mechanism, for which in most intermetallics the transition state theory is applicable. The barrier height entering therein is the difference between the initial equilibrium state and a saddle point state. It is on the latter that traditional treatments have made the most far-reaching simplifying assumptions. Having explored by extensive *ab initio* calculations the actual jump profiles for all jump types eligible and various situations concerning atom environment in Ni_3Al, we discuss the consequences of our results and offer suggestions for an improvement of MC jump rates.

XXXIV. Stochastic statistical theory of nucleation and growth of nano-sized precipitates in alloys with application to precipitation of copper in iron

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Kinetics of nucleation, growh and coarsenig of nano-sized precipitates in alloys is studied basing on the earlier-developed stochastic statistical approach (SSA) with the use of dilute Fe-Cu alloys as an example. Comparison of results of the SSA-based simulation of precipitation employing the simplified direct atomic exchange (DAE) model to the available results of the atomistic Monte Carlo simulation in which a more realistic, vacancy-mediated exchange model is used, shows a good agreement in all microstructural features, including the evolution of sizes, morphology and the number of precipitates, when temporal variations of an effective direct atomic exchange rate due to the vacancy trapping effect are taken into

account, while using the SSA-DAE model reduces the computation time by several orders of magnitude. We also study the dependences of the precipitation kinetics on temperature T and solute concentration c.

We found these dependences to be mainly determined by the reduced supersaturation parameter s= [c-c_b(T)]/[c_s-c_b(T)] where c_b(T) and c_s(T) is the concentration at the binodal and the spinodal, respectively, and at typical s less or of the order of 0.5 these dependences are usually very sharp. We also investigate in detail the kinetics of very first stages of nucleation of nano-sized precipitates and found it to have little in common with the classical nucleation theory notions.

XXXV. Electronic, magnetic, and transport properties of halfmetallic semi-Heusler (Cu,Ni)MnSb alloys

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We report ab initio studies of the electronic structure, finite-temperature magnetism, and transport properties of semi-Heusler quaternary alloys (Cu,Ni)MnSb for a wide range of alloy compositions. Experiments show that the transition from the ferromagnetic state (NiMnSb) to the antiferromagnetic state (CuMnSb) is connected with an abrupt change of the magnetic moments and resistivities at about 70 % Cu concentration while the Curie temperature is a smooth function of the Cu content. We explain this peculiar behavior by the disorder in orientations of the Mn spins that appears at 70 % Cu. A simple account of magnetic disorder within the uncompensated disordered local moment model gives a good quantitative agreement with experimental data.

Poster session

- I. G. M. Bhuiyan *“Entropy of Mixing for AgSn liquid binary alloys”*
- II. L. Isaeva *“Dinamical stability of the defect phase of palladium hydride: ab initio studies”*
- III. E. Kabliman *“Ab initio calculations of formation energies of the Fe-Cr sigma-phase in magnetic state”*
- IV. A. I. Kartsev *“Stability of the face-centered-cubic phases of CoN under pressure”*
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- XIII. L. Pourovskii *“Electronic properties of rare earth monoarsenides and rare earth iron oxyarsenides”*
- XIV. W. Wunderlich *“Ab-initio calculations and experiments on CoSbTi-based Half-Heusler phases for thermoelectric applications”*

PI. Entropy of Mixing for AgSn liquid binary alloys

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The entropy of mixing for Ag_{x}Sn_{1-x} binary alloys has been systematically studied by using the perturbation theory. The interionic interactions as one of the basic ingredients are described by a pseudopotential model in the local form. Since the metals forming the concerned alloys are less simple in nature the effect of the sp-d hybridization is appropriately taken into account through the interionic interactions. Results of calculation across the full range of Ag concentrations are found to be good in agreement with the available experimental data.

PII. Dynamical stability of the defect phase of palladium hydride: ab initio studies

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Studies of the interaction of hydrogen with transition metals and the formation of metal hydrides are of great interest from both fundamental and technological point of view. Without any doubts they are tightly connected with the development of new hydrogen storage and membrane separation materials for hydrogen-based energy technology. Nowadays palladium is one of the most studied material due to its own capability to absorb a plenty amount of hydrogen. Despite of unique properties of Pd-H system, there are limitations of its practical application both in catalytic reactions during hydrogenation and with the storage of hydrogen in crystal volume. The experimental investigations revealed the undesirable changes of atomic structure in palladium matrix caused by hydrogen-metal interaction, which strongly influence on material properties during technological cycles of hydrogen penetration and extraction [1]. The situation is more complicated, when abnormal amount of vacancies (Vac), called superabundant vacancies (SAVs), are induced in palladium during hydrogenation process [2]. The hydrogen induced SAVs lead to the formation of rather stable vacancy-ordered L12 hydride phase, Pd3VacHn, observed recently under different experimental conditions in Pd-H system [3]. However the key role of hydrogen on the formation and composition of this defect structure still remains a challenge. In this work we performed ab initio study of the atomic and electronic properties of vacancy-ordered L12 phase Pd3VacHn of palladium hydride. The thermodynamic stability and composition of this defect structure with regard to various hydrogen concentrations and hydrogen occupation of interstitial sites in palladium are studied systematically. For this purpose we performed the first-principles total energy calculations in the framework of density functional theory [4,5] and pseudopotential approach. Besides, phonon dispersion relations for the defect hydride phase were calculated using the perturbation theory in density functional theory [6] in a wide range of pressure. The obtained results have shown that pressure stabilizes the defect phase for considered hydrogen concentrations. This work was supported by the Russian Foundation for Basic Research (grant N 07-02-01452a).

[1] V.M.Avdukhina, A.A.Anishchenko, A.A.Katsnelson, G.P.Revkevich, Fiz.Tverd.Tela(Leningrad) 47 (2005), 387
[2] Y.Fukai, N.Okuma, Jpn.J.Appl.Phys., Part 2, 32 (1993), L1256
[3] Y.Fukai, N.Okuma, Phys.Rev.Lett. 73 (1994), N12, 1640
[4] P.Hohenberg, W.Kohn, Phys.Rev. 136 (1964), B804
[5] W.Kohn, S.J.Sham, Phys.Rev.B 140 (1965), A1133 [6] P.Gianozzi, S. de Gironcoli, P.Pavone, S.Baromi, Phys.Rev.B 43 (1991) 7231

PIII. Ab initio calculations of formation energies of the Fe-Cr sigma-phase in magnetic state

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In present work sigma-phase in the Fe-Cr alloys was studied using ab initio electronic structure calculations performed by the computer code WIEN2k in the generalized gradient approximation. The aim of investigation is to determine equilibrium state (V, c/a) and formation energies of the Fe-Cr system sigma-phase in ferromagnetic and nonmagnetic state. All calculations are performed in 5 nonequivalent sub-lattice model considering only ordered sigma-phase complexes of ABCDE-form where A, B, C, D, E denotes sub-lattice types. Our simulations show that two ordered sigma-phase configurations FeFeCrFeCr (x(Cr)=0,53) and FeCrFeFeCr (x(Cr)=0,40) in ferromagnetic state are more stable than in paramagnetic one. A value of formation energy calculated relatively bcc-Fe in ferromagnetic state and bcc-Cr in paramagnetic state is lowered especially strong for the FeCrFeFeCr configuration. For both of these sigma-phase complexes equilibrium states (V, c/a) are determined also. It is shown that equilibrium state evaluation needed to be taken into account because it leads to marked decrease of formation energies. Our ab-initio results obtained for the sigma-phase alloys compositions with determined equilibrium parameters in ferromagnetic state are in a satisfactory agreement with experimental data. The research was partially supported by RFBR Project No. 06–03–33152a.

PIV. Stability of the face-centered-cubic phases of CoN under pressure

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Non-magnetic transition metal mononitrides are of great interest materials from both technological and scientific view of points due to their exceptional properties, ranging from superconductivity to hardness, high melting temperature, stability against corrosion. Mostly these nitrides crystallize in the rocksalt (NaCl) structure. But the crystalline structure of equiatomic magnetic metal mononitrides is still under debates. For example, in earlier publications [1-3] it has been reported that CoN adopts either zinc-blend (ZnS) or NaCl-type crystalline structure depending on a method used to synthesize CoN. In this work we study structural, electronic, magnetic, and lattice dynamical properties of CoN phases (NaCl, CsCl, ZnS) in the framework of density functional theory and pseudopotential plane-wave method, as it is implemented in the Quantum Espresso code [4]. Exchange-correlation effects were treated by means of the generalized gradient approximation developed by Perdew-Burke-Ernzerhof [5]. Phonon dispersion modes for CoN phases are obtained using the density functional perturbation method [6]. Our spin-polarized total energy calculations allow us to conclude that NaCl- and ZnS-type CoN phases are nonmagnetic. The calculated ZnS to NaCl phase transition pressure is found to be around 39 GPa. An influence of external pressure in ZnS-type CoN phase is found to be significant, as dynamically stable phase can be destabilized applying small pressure, around 30 kBar.

[1] O. Schmidt-Dumont and N. Kron, Angew. Chem. 67, 231 (1955).
[2] B. Taylor, B. Joyner, and F. H. Verhoek, J. Am. Chem. Soc. 83, 1069 (1961).
[3] K. Suzuki, T. Kaneko, H. Yoshida, H. Morita, H. Fujimori, J. Alloys Compd. 224, 232 (1995).
[4] S. Baroni, A. Dal Corso, S. de Gironcoli, P. Giannozzi, C. Cavazzoni,G. Ballabio, S. Scandolo, G. Chiarotti, P. Focher, A. Pasquarello, K. Laasonen, A. Trave, R. Car, N. Marzari, and A. Kokalj, http://www.pwscf.org/
[5] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett., 77 (1996) 3685.
[6] N. E. Zein, Fiz. Tverd. Tela (Leningrad) 26, 3024 (1984) [Sov. Phys. Tech. Phys. 26, 1825 (1984)]; S. Baroni, S. De Gironcoli, A. Dal Corso, and P. Giannozzii, Rev. Mod. Phys. 73,515 (2001).

PV. Electromigration force on a proton with a bound state

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The driving force on an ion in a metal due to an applied electric field, called the electromigration force, is built up out of two contributions, a wind force and a direct force. The wind force is due to the scattering of the current carrying electrons off the ion. The direct force works on the effective charge of the ion. In the present work we concentrate on the direct force on a migrating proton embedded in an electron gas. For this force a sign change is obtained as soon as a bound state is formed. Recently a bound state was found in a self-consistent potential calculation at lower electron densities. By this the problem has been solved regarding a possible lack of completeness of the published formalism. In earlier calculations no sign change was found. Here we show that a supplementary term shows up, as soon as one accounts for the bound state explicitly. The results presented are based on square-well model potentials. By using different depths it is possible to show results for potentials without a bound state and accomodating one bound state.

PVI. Structural and magnetic properties of Cr telluride-selenide alloys

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We present the results of theoretical study of magnetic and structural properties of Cr telluride-selenide alloys having trigonal crystal structure. Both ground state and temperature-dependent magnetic properties of the Cr$_x$(Te$_\alpha$Se$_\beta$)$_2$ alloys have been investigated in a wide region of $\alpha : \beta$ ratios with various Cr content. Theoretical results are compared with the experimental ones. The ground state properties have been studied on the basis of electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) band structure method. The sub-stoichiometry and the disorder in the chalcogenide sub-lattice has been treated by means of the Coherent Potential Approximation (CPA) alloy theory. The magnetic properties at finite temperature have been studied by means of Monte Carlo simulations on the basis of a classical Heisenberg Hamiltonian and the exchange coupling parameters calculated from first principles. This approach allowed to determine the critical temperature in good agreement with experiment.

PVII. Fe-Ni-C system at high pressure

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Apart from being technologically important, FeNi alloys introduce particularly interest to the material sciences as well as to the geosciences. It is generally accepted that the Earth's core is predominantly composed by FeNi alloy with 10-15 wt% Ni. The certain amount of the light element(s) is also known to be presented in the Core. A number of candidates for the light component have been proposed, including sulphur, oxygen, hydrogen and carbon. In favor of the last one the following arguments can be listed (i) high cosmic abundance, (ii) chemical affinity to iron even at low pressures and (iii) capability of lowering the density of molten iron. Although there is quite a bit of experimental and theoretical results on high pressure high temperature behavior of the system Fe-C, there is still lack of information about the phase relations in Fe-Ni-C system at elevated pressures and temperatures.

Therefore we provided a series of compression experiments on the system Fe-Ni-C at pressures up to 53 GPa in temperature range 300 - 2500 K (combining diamond anvil cell and large volume press techniques) in order to investigate phase diagram of Fe-Ni system and the influence of carbon on the phase relations in the system.

We observed that dissolution of even 1 wt% carbon in FeNi alloys with 10, 15 and 22 wt% Ni leads to dramatic changes in the system: presence of carbon stabilizes *fcc*-structured FeNi through the redistribution of nickel. Combining Mössbauer spectroscopy, XRD, TEM and chemical analyses by microprobe and SEM techniques we detected the formation of Ni-poor and Ni-enriched phases, with different elastic and structural properties.

PVIII. Tuning of magnetic state in high-pressure synthesis of cubic phase in Fe-Si system.

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The importance of the iron-silicon system in metallurgy and geophysics has led to a great number of experimental and theoretical studies concerning the phase equilibrium and properties of phase at different conditions, in particular at high pressure and temperature. It is well known that at ambient pressure Fe and Si produce a large variety of stable bulk binary compounds including FeSi with B20 type of structure, Fe3Si with a DO3 structure with a wide range of stability. As a matter of fact, at intermediate composition Fe2Si alloy is stabilized at high temperature in hexagonal structure. In this paper we show that at high pressure we are able to synthesize cubic phase with Fe2Si composition. The phase has been synthesized at pressure 20 GPa and temperatures between 2300 and 2500 K from Fe-Si mixture using multi-anvil press. The first-principles calculations establish that high pressure - high temperature tuning of magnetic state in Fe-Si system leads to formation of Fe2Si phase with B2 ordering. We carry out calculations of phase stability of Fe2Si alloy by the exact muffin-tin orbitals (EMTO) method in the coherent-potential approximation (CPA) and the Monte Carlo method. Also the effect of influence of a magnetic condition on phase stability is shown.

PIX. Phase stability in disordered alloys: An approach via augmented space recursion based orbital peeling technique

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Orbital peeling technique suggested by Burke peels the orbitals (deletes rows and columns of the Hamiltonian) of the embedded atoms on the averaged medium to determine the small energy differences without involving errors due to subtraction of large numbers. By coupling this technique with augmented space recursion we shall study the phases of the binary disordered alloys and their stability. This approach is capable of providing the effective pair interaction energies accurately enough. Orbital peeling will be carried out in conjunction with the augmented space recursion (ASR) to carry out configuration averaging in disordered systems, coupled with the tight-binding linear muffin-tin orbitals basis (TB-LMTO). Finally we shall describe and analyse our obtained results for different alloy systems. The study will be based on the calculation of effective pair energies obtained through OP. The analysis will involve ordering and mixing energies obtains from a generalized perturbation framework (GPM) and the diffuse scattering intensity, related to the Warren-Cowley parameter, as described by Krivoglatz, Clapp and Moss.

PX. First-principles investigation of multiple hydrogen occupancy of vacancies in Pd

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First-principles investigation of multiple hydrogen occupancy of vacancies in Pd.. In our work we used first principles calculations in order to resolve problems of interaction between hydrogen atoms and vacancies, formation of hydrogen-vacancy complexes and multiple hydrogen occupancy of vacancy. We examined the H-V complexes formation process and occupation of the vacancy by hydrogen atoms. According to our first principles calculations using density functional theory we ascertained that vacancy and hydrogen atoms formed stable complexes. We investigated the process of hydrogen diffusion into the vacancy. We founded the preferable position for hydrogen atom resides in palladium unit cell in the presence of vacancy. We ascertained first that multiple hydrogen occupancy of the monovacancy (up to six hydrogen atoms) is possible. We showed that presence of hydrogen atoms influence on vacancy formation energy and explained the appearance of superabundant vacancy complexes in palladium with absorbed hydrogen.

PXI. Lattice stability of simple metals and phase transitions at ultrahigh pressure

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Progress in the Diamond Anvil Cell technique in tight connection with the use of high-resolution inelastic X-ray scattering beamline made it possible in situ study of high pressure phases. Nowadays, a large amount of experimental data on the phase transition in solid states in megabar pressure range are available. A survey of these data reveals that high pressure phase transitions in simple metals with FCC and BCC lattices are usually transitions to low symmetry phases with formation of new either commensurate or incommensurate phases. In this article we describe the relationship between these phase transitions and high pressure instability of cubic crystalline lattices. We present results of our calculations of the second-order elastic constants for aluminum, vanadium, tantalum, and niobium performed in the framework of density functional theory and in a wide

pressure range. Elastic constants were calculated using volume conserving monoclinic and tetragonal strains. We have shown that inequalities C11 – C12 – 2P >0 and C44 – P >0, where Cij are isothermal elastic constants and P is pressure, are violated in megabar pressure range that results in low symmetry phase transition with shear deformation being the order parameter of these transitions. The deformation phase transitions were considered in the framework of the Landau phase transition theory. This work was supported by the Russian Foundation for Basic Researches (grant # 07-02-01266). All calculations were performed on the Joint Supercomputer Center of the Russian Academy of Sciences.

PXII. A new high pressure high temperature phase of boron.

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Boron is one of the nonmetal elements which physical properties depending on its structure are less described. Because of different combinations of linking of a molecular-like icosahedral cluster boron can exists in at least four structural forms [1-4] known in our days. From the physical point of view, boron becomes the most attractive element due to occurrence of superconductivity at 160 GPa [5], but a structural model of the metallic boron is unknown. By X-ray diffraction patterns we define a new high pressure high temperature (HPHT) phase of boron synthesized using multiavnvil apparatus as well as diamond anvil cell (DAC) technique. From DAC's experiment it was found that a starting material (β-boron) under laser heating can be reversed back through the HPHT modification of boron in the pressure range of 5.8-8 GPa. Under transmission electron microscope (TEM) a regular packing of spheres corresponded to a B_{12} icosahedra was observed. The structure of the HPHT orthorhombic boron was suggested to be consisted of 28 atoms in a unit cell combining two types of icosahedra with four additional inter-icosahedra atoms forming pairs. The structure is certainly novel and unique with Person code of oP28 and Wyckoff sequence of 2h3g. By the near infrared (IR) and optical absorption spectroscopy the synthesized sample is found to be a semiconductor with band gap of 2.1 eV correlated pretty well with calculated by means of first principle modeling value of 1.6-1.7 eV. The negative slope F-f plot with K_0=226 GPa and K'=1.19 was confirmed experimentally (K_{300}=227 GPa, K'=1.2) as well as theoretically (K_0=220-237 GPa, K'=3.6). The highest value of density (2.54 g/cm^3) of the HPHT boron phase from any boron phases can be projected on the hardness of the material. The measured value of H_V is in the range of 35-40 GPa and transfers the synthesized HPHT phase of boron into a superhard class of materials.

[1]. G. Will and B. Kiefer, Z. Anorg. Allg. Chem. 627, 2100-2104 (2001).

[2]. M. Fujimori, T. Nakata, T. Nakayama, E. Nishibori, K. Kimura, M. Takata, and M. Sakata, Phys. Rev. Lett. 82, 22, 4452 (1999).
[3]. V. V. Brazhkin, T. Taniguichi and M. Akaishi, S.V. Popova, J. Mater. Res., Vol. 19, No. 6, 1643 (2004).
[4]. Y. Ma, Ch. T. Prewitt, G. Zou, Ho-kwang Mao, and R. J. Hemley, Phys. Rev. B 67, 174116 (2003). [5]. M. I. Eremets, V. V. Struzhkin, Ho-kwang Mao, R. J. Hemley, Science 293, 272 (2001).

PXIII.Electronic properties of rare earth monoarsenides and rare earth iron oxyarsenides

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We have applied a combination of the dynamical mean-field theory and a first-principles band structure technique to study spectral, thermodynamical, and magnetic properties of several strongly correlated f-electron materials.

In particular, the rare-earth semi-metal ErAs has been investigated. In this compound the Er 4f shell is split by a very strong local Coulomb interaction into the fully occupied and empty parts, which are located well below/above the Fermi level, respectively. Hence the Fermi surface(FS) of this compound is formed by overlapping As 4p and Er 5d bands. However, we demonstrate that a proper treatment of multiplet effects within the Er 4f shell is crucial to obtain correct volume and exchange splitting of the FS as well as for magnetic and spectral properties of this material. By employing an atomic (Hubbard-I) approximation for the strong correlations within the 4f shell we show that the crystal-field splitting of the Er 4f ground state multiplet leads to "freezing" of the Er local magnetic moment and, correspondingly, to a substantial reduction of the FS exchange splitting.

We have also studied the role played by the 4f states in the rare-earth oxyarsenides REOFeAs (RE=Ce,Pr,Nd), where a superconductivity with T$_c$ as high as 50~K has been recently discovered. In the Pr and Nd compounds, the 4f states are located well below and above the Fermi level E_F, and essentially do not interact with the iron 3d bands located near E_F. In the Ce compounds, our results reveal a qualitatively different picture, with the 3d-4f hybridization being sufficiently strong to give rise to an observable Kondo screening and heavy-fermion behaviour. We discuss a possible competition between the supercoducting and heavy-fermion phases in CeOFeAs.

PXIV. Ab-initio calculations and experiments on CoSbTi-based Half-Heusler phases for thermoelectric applications

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One of the candidate for advanced thermoelectric materials are intermetallic Half-Heusler phases on CoSbTi-base or related alloys like NiTiSn, NbNiSn and CoSbZr. Ab-initio simulation using VASP-software could confirm the phase stability against phases with concurrent crystal structures like NiTiSn, CoZrAl, BeZrSi, FeSiV and Full Heusler. For achieving a large Seebeck-coefficent, a large effective mass is essential, which can be estimated from bandstructure calculations as shown previously on doped SrTiO3 [1,2] The results are, that the thermo dynamical driving force for Half Heusler formation as calculated from the difference in lattice energies is less than 0.1eV/atom. Hence, the fabrication of Half heusler phases is difficult and requires three steps, surface activation of the raw material by ball milling, arc-melting of pressed pellets and finally long-term annealing treatment. On doped CoTiSb specimens, Seebeck coefficients up to 0.1 mV/K, on NbNiSb 0.3 mV/K were measured.

[1] W. Wunderlich, K. Koumoto, Int. Jour. Mat. Research 97 (2006) 5 657-662
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