Workshop on

ATOMIC-SCALE CHALLENGES IN ADVANCED MATERIALS

Materials research - combing theory and experiments

June 11th - June 12th, 2015
Turku, Finland

organized by
Materials Physics Group and Turku University Centre for Materials and Surfaces (MatSurf)
University of Turku

Max Planck Institute of Microstructure Physics &
Martin Luther University Halle-Wittenberg

Contents

Program 3

Abstracts: 8

Theory and methods . . . 8
Structure and magnetism . . . 12
Functional oxides for applications . . . 16
Stability and equilibrium properties of alloys I . . . 22
Stability and equilibrium properties of alloys II . . . 26
High entropy alloys . . . 30
Nanostructures . . . 34

List of participants 39

Organization committee 43

Notes 45

Program

Thursday: June 11th, 2015

10:00-10:20	OPENING SESSION (Prof. Petriina Paturi)	

Theory and Methods: (Prof. Wolfram Hergert)

10:20-10:40	Agnes Nagy	*Pauli Potential in the Density and Pair Density Functional Theories*
10:40-11:00	Matthias Geilhufe	*Implementation of a relativistic full-potential KKR method and a numerical discussion for the Mathieu potential*
11:00-11:20	Alberto Marmodoro	*Revisiting the NLCPA: insight from non-site-diagonal observables*
11:20	CONFERENCE PICTURE Outside	
11:30-13:30	LUNCH at Cafeteria Macciavelli	

Structure and Magnetism: (Prof. Kalevi Kokko)

13:30-13:50	Dongyoo Kim	*Induced twinning deformation in Al by compressed volume and lattice distortion*
13:50-14:10	Andreas Östlin	*Origin of β-Cerium investigated with ab initio calculations of stacking fault energies*
14:10-14:30	Kurt Gloos	*Electron-Spectroscopic Characterization of metal Interfaces*
14:30-14:50	Zhihua Dong	*Thermal Spin Fluctuation in Paramagnetic Fe and Stainless Steel Fe15Cr15Ni from First-Principles*
14:50-15:30	COFFEE BREAK	

Functional Oxides for Applications: (Prof. Petriina Paturi)

15:30-15:50	Waheed Adeagbo	*Strain effects and defect study on Sr_2FeMoO_6 bulk and films from first-principles*
15:50-16:10	Sanjeev Kumar Nayak	*Comparative study of isolated Li defects and V Zn–Li defect complexes in ZnO*
16:10-16:30	Martin Hoffmann	*Room temperature magnetism in Zn-ferrite due to structural defects*
16:30-16:50	Tomi Elovaara	*Magnetophotoresistance in the $Pr_{1-x}Ca_xMnO_3$ thin films*
16:50-17:10	Sari Granroth	*Photoelectron Spectroscopy of $Pr_{1-x}Ca_xMnO_3$ and Sr_2FeMoO_6 Perovskite Thin Films*
19:00-21:00	CONFERENCE DINNER at Restaurant Ship Svarte Rudolf	

Friday: June 12th, 2015

Stability and Equilibrium Properties of Alloys I: (Prof. Levente Vitos)

9:00-9:20	Song Lu	*On the tetragonality of martensites in Fe_3Pt alloys: an ab initio study*
9:20-9:40	Stephan Schönecker	*Metastable cubic and tetragonal phases of transition metals predicted by density-functional theory*
9:40-10:00	Li-Yun Tian	*Elastic constants of random fcc Ti-Al alloy from SQS and CPA calculations*
10:00-10:30		COFFEE BREAK

Stability and Equilibrium Properties of Alloys II: (Prof. Levente Vitos)

10:30-10:50	Wei Li	*Generalized Stacking Fault of γ-Fe and It's Alloys*
10:50-11:10	Henrik Levämäki	*An EMTO database of elastic constants for pure elements*
11:10-11:30	Guisheng Wang	*On the ab initio prediction of the mechanical properties of alloys: The case of Ni/Mn-doped ferromagnetic Fe*
11:30-11:50	Ruihuan Li	*Stability of a single He in interstitial sites of $Fe_{1-x}Cr_x$ alloys: A first-principles study*
11:50-13:30		LUNCH at Cafeteria Macciavelli

High Entropy Alloys: (Dr. Stephan Schönecker)

13:30-13:50	Xiaoqing Li	*Ab initio-predicted micro-mechanical performance of refractory high-entropy alloys*
13:50-14:10	Shuo Huang	*Temperature dependent Stacking Fault Energy of FeCrCoNiMn High Entropy Alloy*
14:10-14:30	Lajos Varga	*Designing high entropy alloys based on the tabulated physical properties of the constituent elements*
14:30-15:00		COFFEE BREAK

Nanostructures: (Prof. Agnes Nagy)

15:00-15:20	Sayani Majumdar	*Effect of bottom electrodes on the tunneling electro-resistance in P(VDF-TrFE) based hybrid ferroelectric tunnel junctions for non-volatile memories*
15:20-15:40	Wolfram Hergert	*Properties of 3d transition metal point defects used to stabilize hexagonal $BaTiO_3$ at room temperature*
15:40-16:00	Antti Kuronen	*Simulation of nanoindentation of gold nanorods*
16:00-16:20	Ville Polojärvi	*Defects in Dilute Nitride Solar Cells*
16:20-16:40		CLOSING

Abstracts:
Theory and methods

Thursday, June 11th, 10:20-10:40

Pauli Potential in the Density and Pair Density Functional Theories

• Ágnes Nagy

Department of Theoretical Physics, University of Debrecen, Hungary

A link between density and pair density functional [1] theories is presented. Density and pair density scaling [2,3] are used to derive the Euler equation in both theories. Density scaling provides a constructive way of obtaining approximations for the Pauli potential [4]. The Pauli potential (energy) of the density functional theory is expressed as the difference of the scaled and original exchange-correlation potentials (energies). A relationship between the effective potentials of the Euler equation of the density functional theory and the Pauli potential of the pair density functional theory is also presented [5].

References

[1] Á. Nagy, Phys. Rev. A **66**, 022505 (2002)
[2] G. K.-L. Chan and N. C. Handy, Phys. Rev. **59**, 2670 (1999)
[3] Á. Nagy, J. Chem. Phys. **123**, 044105 (2005)
[4] Á. Nagy, Phys. Rev. A **84**, 032506 (2011)
[5] Á. Nagy, Comp. Theor. Chem. **1003**, 97 (2013)

Thursday, June 11th, 10:40-11:00

Implementation of a relativistic full-potential KKR method and a numerical discussion for the Mathieu potential

• Matthias Geilhufe [1] Steven Achilles [2] Markus Arthur Köbis [3] Martin Arnold [3] Ingrid Mertig [1,2] Wolfram Hergert [2] Arthur Ernst [1]

[1] *Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*
[2] *Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany*
[3] *Institute of Mathematics, Martin Luther University Halle-Wittenberg, Germany*

For the implementation of a fully-relativistic full-potential Korringa-Kohn-Rostoker Green function method, an accurate solution of the single-site scattering problem is

necessary. Within this talk an implementation of a solver for the single-site scattering problem will be discussed, first, by means of the direct solution of the underlying differential equations and, second, by means of the solution of the Lippmann-Schwinger equation. Furthermore the numerical accuracy for the Mathieu potential [1] will be compared. Instead of using the Lippmann-Schwinger equation like in previous implementations [2,3], it will be shown, that the solution via linear multi-step methods is a reasonable choice. In particular, an Adams-Bashforth-Moulton predictor-corrector method was implemented within the KKR code Hutsepot and it will be used to compare analytical and numerical band structure calculations.

References

[1] C.-Y. Yeh *et al.*, Phys. Rev. B **42**, 10976-10982 (1990)
[2] B. Drittler *et al.*, Solid State Commun. **79**, 31-35 (1991)
[3] T. Huhne *et al.*, Phys. Rev. B **58**, 10236-10247 (1998)

Thursday, June 11th, 11:00-11:20

Revisiting the NLCPA: insight from non-site-diagonal observables

• Alberto Marmodoro [1] A. Ernst [1] L. Sandratskii [1] P. Trevisanutto [2] J.B. Staunton [3]

[1] *Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*
[2] *Singapore Synchrotron Light Source, National University of Singapore, 5 Research Link, Singapore 117603*
[3] *Department of Physics, University of Warwick, CV4 7AL Coventry, United Kingdom*

We re-examine the non-local coherent potential approximation (NLCPA) from the point of view of actual unicity in its effective medium construction.
This method extends the originally single-site theory [1] with the ability of modelling different forms of short-range ordering (SRO) [2]. Characteristically with respect to other extension proposals [3], in this approach to the study of disordered systems on-average translational invariance is retained. This derives from a self-consistent prescription which couples extended treatment in direct space (i.e. a $N_c \geq 1$ -sites wide 'cavity' carved from the bulk) with a Brillouin zone partitioning in reciprocal space (i.e. $N_c \geq 1$ 'tiles' $\boldsymbol{\Omega}_{BZ}^{(cav)}(\boldsymbol{K}_n)$ such that: $\bigcup_{n=1}^{N_c} \boldsymbol{\Omega}_{BZ}^{(cav)}(\boldsymbol{K}_n) = \boldsymbol{\Omega}_{BZ}$).
After iterating between both descriptions until convergence, results can be used for the actual calculation of all desired observables. As in the original theory [4], it is convenient to distinguish in particular among site-diagonal (SD) and non-site-disagonal (NSD) quantities. Essential examples of these can be the electronic density of states, as opposed to the electronic Bloch's spectral function which corresponds to its $\boldsymbol{k} \in \boldsymbol{\Omega}_{BZ}$ derivative.

We show how proper deployment of the general formalism to calculate the latter at a Korringa, Kohn, Rostocker (KKR) -DFT level for real materials [5] confirms previous insight from 1D tight-binding calculations [6]. The role of a "free" phase factor in the above lattice Fourier transformations definition becomes in particular apparent, with noticeable consequences in both SD and NSD observables. This requires in general an extra averaging step for recovery of a fully physical effective medium. We review this additional aspect of the theory and re-look at previous case studies in the physics of substitutional alloys, as well as disordered local moment simulations of the paramagnetic phase of metals, for different forms of spectroscopy [7-9] are available

References

[1] Soven, PR **156**, 809-813 (1967)
[2] Rowlands *et al.*, PRB **67(11)**, 1-9 (2003)
[3] Rowlands, JPCM **18**, 3179 (2006)
[4] Faulkner *et al.*, PRB **21(8)**, 3222-3244 (1980)
[5] Tulip *et al.*, PRB **73(20)**, 1-12 (2006)
[6] Rowlands *et al.*, PRB **78(11)**, 115119 (2008)
[7] Kirschner *et al.*, PRL **53(6)**, 612-615 (1984)
[8] Kisker *et al.*, PRB **31(1)**, 329-339 (1985)
[9] Brown *et al.*, JMMM **30(2)**, 243-248 (1982)

Abstracts: Structure and magnetism

Thursday, June 11th, 13:30-13:50

Induced twinning deformation in Al by compressed volume and lattice distortion

• Dongyoo Kim [1] Levente Vitos [1,2,3]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*
[3] *Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary*

We investigate plastic deformation behavior of faced center cubic (FCC) Al under compressed volume and lattice distortion via first principles. Competition between slip and twin barriers is dealt as main mechanism of plastic deformation, and this is well described in plastic deformation map (PDM) [1]. We observe that generalized stacking fault energy (GSFE), consisted with intrinsic, extrinsic, unstable stacking fault energy and unstable twinning fault energy, linearly depend on volume and lattice distortion, but their change as a function of volume and lattice distortion is not same. Based on PDM and observed GSFEs, we find that volume and lattice distortion effectively modify the plastic deformation behavior, and twinning deformation in Al can be induced by compressed volume and lattice distortion.

References

[1] Jo *et al.*, Proc. Natl. Acad. Sci. **111**, 6560 (2014)

Thursday, June 11th, 13:50-14:10

Origin of β–cerium investigated with *ab initio* calculations of stacking fault energies

• Andreas Östlin [1] Jason C. Lashley [2,3] Levente Vitos [1,2,4]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Los Alamos National Laboratory, P.O. Box 1663 Bikini Atoll Road, Los Alamos, New Mexico, USA*
[3] *Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary*

At zero pressure the element cerium shows a metastable ($t_{1/2} \sim 40$ years) double hexagonal close-packed β-phase that is positioned between two cubic phases, γ and α. With modest pressure the β-phase can be suppressed, and a volume contraction (17 %) occurs between α and γ phases as temperature is varied. This phenomena has been linked to subtle alterations in the $4f$ band. In order to rationalize the presence of the metastable β-phase, and its position in the phase diagram, we have computed stacking fault formation energies of the cubic phases of cerium. It is found that there is a large difference in the stacking fault energies between the α and γ-phase. The β-phase energy is nearly degenerate with the γ-phase, and can be seen as a dislocation reservoir that appears to be necessary to accommodate the large strains generated during the α-γ transition. Such a degeneracy explains long standing third law calorimetry results, and dislocation dynamics the pressure and temperature hysteretic effects.

Thursday, June 11th, 14:10-14:30

Electron-Spectroscopic Characterization of Metal Interfaces

• Kurt Gloos

Department of Physics and Astronomy, University of Turku, Finland

The quality of metal interfaces can be investigated by observing how they scatter electrons or holes. Electron-phonon spectroscopy uses the spectral intensity of back-scattered electrons to estimate the amount of elastic scattering in the contact region. Andreev-reflection spectroscopy at superconductor - normal metal interfaces employs the Andreev reflected holes from inside the superconductor that are transmitted through or reflected at the contact interface to determine the reflection or transmission coefficient. The two methods yield contradictory results: Andreev reflection indicates that practically all metal interfaces are diffusive (that is they contain a certain amount of disorder or defects at which electrons or holes are scattered), independently of whether electron-phonon spectroscopy shows that the same interfaces are diffusive or ballistic [1].
Both methods have their drawbacks. The phonon density of states in the contact region can deviate from that of the bulk metal, blurring the spectral features and, thus, simulate more diffusion. On the other hand, one can under-estimate the Andreev-derived normal reflection by neglecting electronic, thermal, or lifetime broadening. Luckily these error mechanisms affect the true normal reflection oppositely and therefore do not diminish the above mentioned main result that ballistic contacts are at the same time diffusive.
How reliable is the value of the normal reflection as measured by Andreev reflection spectroscopy? In the ideal case the Andreev-reflection spectra are fitted with only three adjustable parameters: superconducting energy gap 2Δ, normal reflection parameter Z, and Dynes' lifetime parameter Γ. This allows to determine the normal

reflection coefficient to within one percent. Since the contacts are - according to our interpretation - diffusive, we have to consider a distribution of transmission coefficients, that is each of the many conductance channels or modes i of an interface has its own coefficient $\tau_i = 1/(1 + Z_i^2)$. The distribution itself is unknown except some ideal theoretical cases. Other parameters like an effective temperature might be taken into account, but all this leads to different parameter sets, including the reflection parameter, that describe almost equally well the experimental data. We discuss possible ways to reduce this ambiguity.

References

[1] K. Gloos and E. Tuuli, Low Temp. Phys. **40**, 902 (2014)

Thursday, June 11th, 14:30-14:50

Thermal Spin Fluctuation in Paramagnetic Fe and Stainless Steel Fe15Cr15Ni from First-Principles

• Zhihua Dong

Department of Materials Science and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden

The great variety intrinsic properties of Fe and its alloys are dependent on the magnetic state of it. At thermal excitations, the atomic moment or spin fluctuation becomes an important question in itinerant-electron systems. In the present work, the spin fluctuation distribution is established using Boltzmann statistical scheme based on series constrained local magnetic moment modelings. The temperature dependence of elastic constants (c' and c_{44}) of paramagnetic (PM) bcc Fe, fcc Fe, and fcc Fe15Cr15Ni are investigated under thermo-magneto-volume coupling with the consideration of spin fluctuation. According to the theoretical predictions, in PM bcc Fe, the spin fluctuation tends to improve the decreasing rate of elastic constants when the temperature increases; and it slows down the decreasing process in fcc Fe and austenitic stainless steel Fe15Cr15Ni. With respect to pure fcc Fe, spin fluctuation has greater contributions to the elastic properties of stainless steel Fe15Cr15Ni. At 1600 K, the decreasing rate of c' and c_{44} contributed from volume expansion could be canceled out by about 40 % and 10 %, respectively, by thermal spin fluctuation in Fe15Cr15Ni.

Keywords: Spin fluctuation; paramagnetic Fe; austenitic stainless steel Fe15Cr15Ni; elastic constants; temperature

Abstracts: Functional oxides for applications

Thursday, June 11th, 15:30-13:50

Strain Effects and Defect Study on Sr_2FeMoO_6 Bulk and Films from First-Principles

• Waheed A. Adeagbo [1] Martin Hoffmann [1,2] Arthur Ernst [2]
Wolfram Hergert [1] Minnamari Saloaro [3] Petriina Paturi [3]

[1] *Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany*
[2] *Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*
[3] *Wihuri Physical Laboratory, Department of Physics and Astronomy, University of Turku, Finland*

Spin polarized half-metallic ferromagnetic complex oxides like double perovskite Sr_2FeMoO_6 (SFMO) have attracted intensive interest in materials science. They are considered as a good material for creating spin-polarized current for next-generation spintronics devices especially as magnetic tunnel junctions (MTJs). The Curie temperature, T_C, in its bulk state is exceptionally high, around 410 K to 450 K [1]. For potential application, we need thin films rather than polycrystalline or bulk samples. Therefore, the production of high quality thin films with high T_C and magnetic properties close to the bulk material is desired but hindered by various imperfections such as anti-site disorder (ASD), oxygen vacancies (V_O) or epitaxial strain during the growth process.

To investigate some of these imperfections, we have carried out first-principles calculations based on the density functional theory using the pseudo-potential code, Vienna *ab initio* simulation package (VASP), with the implemented projector augmented wave (PAW) method and the on-site Coulomb interaction correction taken into account with PBE+U [2].

The order of defects or the stability of imperfections are classified with respect to their formation energies. We investigated the role of biaxial strains which might result from the lattice mismatch of the various substrates on which the SFMO films are grown. Concerning possible applications, the half-metallic character of SFMO with its high spin polarization is crucial. In the bulk, this is still preserved for a small strain or the presence of V_O in agreement with previous *ab initio* calculations [3]. The magnetic moment reduction of $2\,\mu_B$ per vacancy is also observed for V_O. In contrast, ASD alone or together with an V_O as a defect complex reduces the spin polarization. In agreement with experiment, the slab calculations show the presence of compressive strains which decrease with increasing film thickness.

References

[1] K. I. Kobayashi *et al.*, Nature **395**, 677 (1998)
[2] G. Kresse *et al.*, Phys. Rev. B **47**, 558 (1993)
[3] A. B. Muñoz-García *et al.*, Chem. Mater. **32**, 4525 (2011)

Thursday, June 11th, 15:50-16:10

First-principles study of Li defect complexes in ZnO

• Sanjeev K. Nayak [1] Israel V. Lorite [2] Pablo D. Esquinazi [2]
Wolfram Hergert [1]

[1] *Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle, Germany*
[2] *Division of Superconductivity and Magnetism, Institute for Experimental Physics, University of Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany*

A recent experimental study on proton-implanted Li-doped ZnO microwires has shown room temperature ferromagnetic property. X-ray magnetic circular dichroism (XMCD) spectrum shows peaks at O K-edge, suggesting spin-polarization in O atoms. A comparison of measured XMCD specta and simulated spectra by first-principles method shows that the magnetic signal is mainly due to presence of Zn vacancies (V_{Zn}) in the sample [1]. Similar conclusion has been derived earlier [2]. This gives rise to the hypothesis that Li doping helps in stabilizing V_{Zn}. In order to verify the hypothesis we carry out density functional theory (DFT) investigations on Li-doped ZnO system. The stability of defect complexes is analysed by estimating their formation energies at various partial pressure of oxygen atmosphere (see Ref. 3). In order to overcome the limitations of DFT we use empirical postprocessing treatment [4] and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional approach [5]. Our results show that Li in ZnO favors an interstitial position both as an isolated defect and as a defect complex. The charge transition level (+2/+) of Li interstitial is found to lie in the band gap at 50 meV above the valence band maximum. This suggests that *p*-type condition could be possible in Li-doped ZnO.

References

[1] I. Lorite *et al.*, Appl. Phys. Lett. **106**, 082406 (2015)
[2] J. B. Yi *et al.*, Phys. Rev. Lett. **104**, 137201 (2010)
[3] S. K. Nayak *et al.*, Phys. Rev. B **91**, 155105 (2015)
[4] S. Lany and A. Zunger, Phys. Rev. B **78**, 235104 (2008)
[5] J. Heyd *et al.*, J. Chem. Phys. **118**, 8207 (2003)

Thursday, June 11th, 16:10-16:30

Room temperature magnetism in Zn-ferrite due to structural defects

• M. Hoffmann [1,2] S. K. Nayak [1] W. A. Adeagbo [1]
K. L. Salcedo Rodríguez [3] C. E. Rodríguez Torres [3]
Arthur Ernst [2] W. Hergert [1]

[1] *Martin Luther University Halle-Wittenberg, Institute of Physics, Von-Seckendorff-Platz 1, 06120 Halle, Germany*
[2] *Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*
[3] *Departamento de Física, Facultad de Ciencias Exactas, C. C. 67, National University of La Plata, 1900 La Plata, Argentina*

Cation site inversion between regular and inverse spinel compositions and oxygen vacancy (V_O) mediated ferromagnetic coupling between Fe spins constitute two major physical mechanisms for the observed ferrimagnetism in $ZnFe_2O_4$ (ZFO) at room temperature [1]. This conclusion is based on experimental results from x-ray magnetic circular dichroism measurements at the Fe $L_{2,3}$ edges and magnetization measurements performed on zinc ferrite nanoparticles and films, with different cation distributions and oxygen vacancy concentrations. Our density-functional-theory calculations indicate that the enhanced ferrimagnetic response observed in some nominally nonmagnetic or antiferromagnetic ferrites can be taken as a further example of the defect-induced magnetism phenomenon. Therefore, we studied the magnetic coupling between the Fe ions in ZFO with and without V_O in more detail. The formation energy of defects is used to analyze the stability of V_O in ZFO for the experimental growth conditions. The Néel temperature (T_N) is determined from Monte Carlo (MC) simulations using the magnetic exchange interactions (J_{ij}) obtained from first-principles method. The correlation energy is treated using GGA+U, where it is found that the J_{ij} change almost linearly with increasing values of U. For T_N comparable to the experimental results, the first neighbor interaction was small and positive as concluded from former experiments. With those J_{ij}, the estimated temperature-dependent saturation magnetization from the MC simulations is in good agreement with recent measurements.

References

[1] C. E. Rodríguez Torres *et al.*, Phys. Rev. B **89**, 104411 (2014)

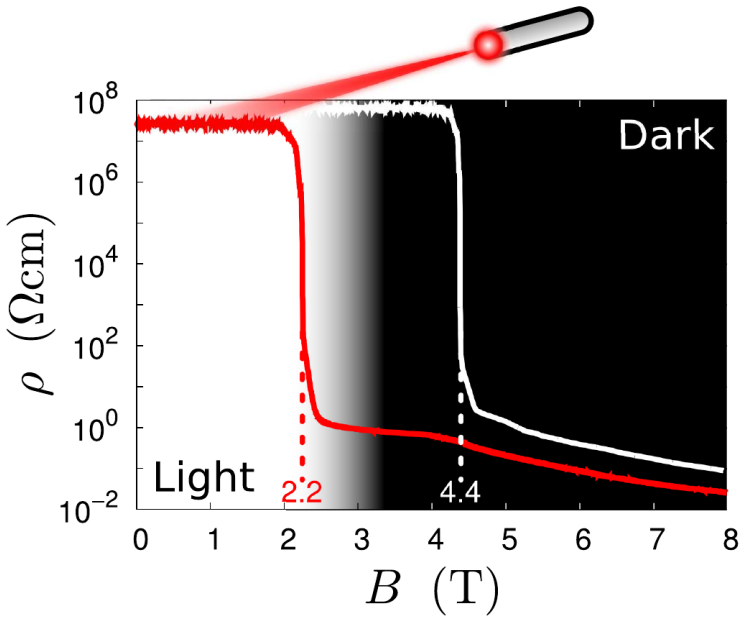
Thursday, June 11th, 16:30-16:50

Magnetophotoresistance in $Pr_{1-x}Ca_xMnO_3$ Thin Films

• Tomi Elovaara [1] S. Majumdar [1,2] H. Huhtinen [1] P. Paturi [1]

[1] *University of Turku, Department of Physics and Astronomy, FI-20014 Turku, Finland*
[2] *Aalto University School of Science, P.O. Box 15100, FI-00076 Aalto, Finland*

The colossal magnetoresistive insulator to metal switching of almost nine orders of magnitude under the significantly reduced magnetic field is achieved by illumination for the low bandwidth manganite thin films. Similarly, by changing the measuring bias voltage through the sample the required magnetic field for insulator-metal transition can be further fine-tuned. By applying a magnetic field of suitable strength, the samples can also be tuned to be extra sensitive to the illumination having colossal effect on the resistivity at low temperatures. This kind of utilizing of multiple external stimulants, which together change the properties of the material could have significant impact on the new generation of phase-change memories working under affordable conditions.



Thursday, June 11th, 16:50-17:10

Photoelectron Spectroscopy of $Pr_{1-X}Ca_xMnO_3$ and Sr_2FeMoO_6 Perovskite Thin Films

• Sari Granroth [1] Tomi Elovaara [2] Minnamari Saloaro [2] Hannu Huhtinen [2] Jussi Tikkanen [2] Petriina Paturi [2]

[1] *Department of Physics and Astronomy, Laboratory of Materials Research, Vesilinnantie 5, FIN-20014 University of Turku, Finland*

[2] *Department of Physics and Astronomy, Wihuri Physical Laboratory, Vesilinnantie 5, FIN-20014 University of Turku, Finland*

$Pr_{1-x}Ca_xMnO_3$ (PCMO) and Sr_2FeMoO_6 (SFMO) perovskite oxide films have several interesting properties related to hybrid spintronic devices and applications of magnetoresistive materials, which offer more functionality and performance than the conventional solutions. It is known that the ferromagnetic double exchange interaction in mixed valence manganites (PCMO) is extremely sensitive to the Mn^{3+}/Mn^{4+} ratio which was investigated as a function of Ca concentration (x) and temperature. The fabrication of SFMO thin films is difficult due to easily formed impurity phases, oxygen non-stoichiometry and antisite disorder, where Fe and Mo ions swap their places in the structure. We have used Hard X-ray Photoelectron Spectroscopy (HAXPES) to carry out bulk sensitieve studies of PCMO and SFMO to better understand these phenomena and the electronic structure of the thin films.

Abstracts: Stability and equilibrium properties of alloys I

Friday, June 12th, 9:00-9:20

On the tetragonality of martensites in Fe_3Pt alloys: an *ab initio* study

• Song Lu [1] Qing-Miao Hu [2] Levente Vitos [1,3,4]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*
[3] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*
[4] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

The effects of point defects on the tetragonality of martensitic phases in Fe_3Pt alloys are studied with *ab initio* methods. We show the great effects of different point defects on rendering the Bain path.

Friday, June 12th, 9:20-9:40

Metastable cubic and tetragonal phases of transition metals predicted by density-functional theory

• Stephan Schönecker

Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden

By means of density-functional calculations, we systematically investigated 24 transition metals for possible metastable phases in body-centered tetragonal structure (bct), including face-centered cubic (fcc) and body-centered cubic (bcc) geometries. A total of 36 structures not coinciding with equilibrium phases were found to minimize the total energy for the bct degrees of freedom. Among these, the fcc structures of Sc, Ti, Co, Y, Zr, Tc, Ru, Hf, Re, and Os, and bct Zr with $c/a = 0.82$ were found to be metastable according to their computed phonon spectra. Eight of these predicted phases are not known from the respective pressure-temperature phase diagrams. Possible ways to stabilize the predicted metastable phases are illustrated.

Friday, June 12th, 9:40-10:00

Elastic constants of random fcc Ti-Al alloy from SQS and CPA calculations

• Li-Yun Tian [1] Qing-Miao Hu [2] Levente Vitos [1,3,4]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*

[2] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*

[3] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*

[4] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

Special quasi-random structure (SQS) and coherent potential approximation (CPA) are techniques widely employed in the first-principles calculations of random alloys. Here we scrutinize these approaches by focusing on the local lattice distortion (LLD) and the crystal symmetry effects. We compared the lattice parameters, mixing energy, and elastic constants obtained from SQS and CPA calculations, taking the random face-centered cubic (fcc) $Ti_{1-x}Al_x$ ($0 \leq x \leq 1$) alloy as example. For the CPA and SQS calculations, we employ the Exact Muffin-Tin Orbitals (EMTO) method and the pseudopotential method as implemented in the Vienna Ab initio Simulation Package (VASP), respectively. We show that the composition dependences of the VASP-SQS and EMTO-CPA parameters are in good agreement with each other. The energy associated with the LLD increases with x up to $x = 0.625$ to 0.750 and drops drastically thereafter. The influence of the LLD on the lattice constants, mixing energy, and c_{12} elastic constant is negligible. c_{11} and c_{44} decrease after atomic relaxation for alloys with large LLD, however, the trends of c_{11} and c_{44} are not significantly affected. In general, the uncertainties associated with the symmetry lowering turn out to be superior to the differences between the two techniques including the effect of LLD.

Abstracts: Stability and equilibrium properties of alloys II

Friday, June 12th, 10:30-10:50

Generalized stacking fault energy of γ-Fe

• Wei Li [1] Song Lu [1] Qing-Miao Hu [2] Börje Johansson [1,3]
Se Kyun Kwon [4] Mikael Grehk [5] Jan Y. Johnsson [6]
Levente Vitos [1,3,7]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*
[3] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*
[4] *Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 790-784, Korea*
[5] *AB Sandvik Materials Technology, SE-811 81 Sandviken, Sweden*
[6] *Outokumpu Stainless AB, Avesta Research Centre, SE-774 22 Avesta, Sweden*
[7] *Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary*

We investigate the generalized stacking fault energy of paramagnetic γ-Fe as a function of temperature. At static conditions, the face centered cubic lattice is unstable with respect to the hexagonal close packed lattice, resulting in negative intrinsic stacking fault energy (ISF) and large positive unstable stacking fault energy (USF). The ISF has a strong positive temperature coefficient, turning positive around 300 K. The USF decreases monotonously with temperature. According to the recent plasticity theory, the overall effect of temperature is to move the system from the stacking fault formation regime ($T \ll 300\,\mathrm{K}$) towards maximum twinning ($T \approx 300\,\mathrm{K}$) and finally to a dominating full-slip regime ($T \gg 300\,\mathrm{K}$).

Friday, June 12th, 10:50-11:10

An EMTO database of elastic constants for pure elements

• Henrik Levämäki

Department of Physics and Astronomy, University of Turku, FI-20014 Turku, Finland
Turku University Centre for Materials and Surfaces (MatSurf), Turku, Finland

The elastic constant tensor, along with the volume and the bulk modulus, is fundamental to the understanding of mechanical properties of materials. Elastic constants

provide insight into the bonding in the material and they also correlate with many macroscopic mechanical properties, such as ductility, brittleness, and hardness. In this light, it is interesting to note that only a couple of systematically computed elastic constant databases have been reported [1,2] and they are both limited to the same computational method (projector-augmented wave method as implemented in VASP). To compare different computational methods and to verify the results of the previous databases, we have calculated the elastic constants of a large set of pure elements using the exact muffin-tin orbitals method (EMTO). Elastic constants of pure elements are often needed when modeling multicomponent systems e.g. through the CALPHAD approach. To handle the large workload, modern many-task computing and automation approaches [2-5] have been utilized. This database will form a part of the basis for future projects, such as modeling and understanding high-entropy alloys and other multicomponent systems.

References

[1] Shang, S.L. *et al.*, Comp. Mater. Sci. **48**, 813 (2010)
[2] de Jong, M. *et al.*, Nat. Sci. Data , (2015)
[3] Curtarolo, S. *et al.*, Nat. Mater. **12**, 191 (2013)
[4] Shyue, P.O. *et al.*, Comp. Mater. Sci. **68**, 314 (2013)
[5] Levämäki *et al.*, pyEMTO toolkit , (2015)

Friday, June 12th, 11:10-11:30

On the *ab initio* prediction of the mechanical properties of alloys: The case of Ni/Mn-doped ferromagnetic Fe

• Guisheng Wang [1] Stephan Schönecker [1] Staffan Hertzman [2]
Qing-Miao Hu [3] Börje Johansson [1,4] Se Kyun Kwon [5]
Levente Vitos [1,4,6]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*
[2] *Department of Materials Science and Engineering, Outokumpu Stainless Research Foundation, Royal Institute of Technology, Stockholm SE-100 44, Sweden*
[3] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*
[4] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*
[5] *Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 790-784, Korea*
[6] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

First-principles alloy theory, formulated within the exact muffin-tin orbitals method in

combination with the coherent-potential approximation, is used to study the mechanical properties of ferromagnetic body-centered cubic (bcc) $Fe_{1-x}M_x$ alloys (M = Mn or Ni, $0 \leq x \leq 0.1$). We consider several physical parameters accessible from *ab initio* calculations and their combinations in various phenomenological models to compare the effect of Mn and Ni on the properties of Fe. Alloying is found to slightly alter the lattice parameters and produce noticeable influence on elastic moduli. Both Mn and Ni decrease the surface energy and the unstable stacking fault energy associated with the $\{110\}$ surface facet and the $\{110\}\langle 111\rangle$ slip system, respectively. Nickel is found to produce larger effect on the planar fault energies than Mn. The semi-empirical ductility criteria by Rice and Pugh consistently predict that Ni enhances the ductility of Fe but give contradictory results in the case of Mn doping. The origin of the discrepancy between the two criteria is discussed and an alternative measure of the ductile-brittle behavior based on the theoretical cleavage strength and single-crystal shear modulus $G\{110\}\langle 111\rangle$ is proposed.

Keywords: magnetism; elastic constants; surface energy; stacking fault energy

Friday, June 12th, 11:30-11:50

Stability of a single He in interstitial sites of $Fe_{(1-x)}$-Cr_x alloys: A first-principles study

• Ruihuan Li [1] Levente Vitos [1,2,3]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden*

[2] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*

[3] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

The Low-activated ferritic/martensitic steels are proposed as structural material in fusion reactors due to its greatest maturity in technology. In fusion environment, huge amounts of He atoms are produced by transmutation along with structural damage in the structural materials. The production of insoluble He is a special issue for the fusion environment and therefore an important problem in the design of fusion reactor. Using density-functional theory in combination with the exact muffin-tin orbital (EMTO) as well as vienna *ab initio* simulation package (VASP), we have calculated the total energies of a single He in bcc Fe supercell of 16 atoms ($2 \times 2 \times 2$) as function of volume of supercell. The two methods give the same energy trend with increasing the volume of supercell and also give the same energy difference between two different volumes. Based on this result, we further investigated the alloy effect on the stability of single He atom in interstitial sites by EMTO. Our results show the formation energies of a single He in interstitial sites increase with increasing Cr content in $Fe_{(1-x)}$-Cr_x alloys (x = 0, 0.09, 0.15, 0.5, 0.95, 1).

Abstracts: High entropy alloys

Friday, June 12th, 13:30-13:50

Ab initio predicted micro-mechanical performance of refractory high-entropy alloys

• Xiaoqing Li

Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden

Recently developed high-entropy alloys (HEAs) consisting of multiple principal elements represent a new field of metallurgy and have demonstrated appealing properties for a wide range of applications. Using *ab initio* alloy theory, we reveal the alloying effect on the elastic properties and the ideal tensile strength (ITS) in the [001] direction of four body-centered cubic (bcc) refractory HEAs based on Zr, V, Ti, Nb, and Hf. We find that these HEAs show high elastic anisotropy and large positive Cauchy pressure, suggesting good extrinsic ductility. Starting from ZrNbHf, it is found that the ITS decreases with equimolar Ti addition. On the other hand, if both Ti and V are added to ZrNbHf, the ITS is enhanced by about 42 %. An even more captivating effect is the ITS increase by about 170 %, if Ti and V are substituted for Hf. The alloying effect on the ITS is explained by the d-band filling. A brittle-to-ductile transition is found in terms of the failure-mode under uniaxial tension. These investigations suggest that intrinsically ductile HEAs with high ideal strength can be achieved by controlling the proportion of group four elements to group five elements.

Friday, June 12th, 13:50-14:10

Temperature dependent Stacking Fault Energy of FeCrCoNiMn High Entropy Alloy

• Huang Shuo

Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-10044, Sweden

The stacking fault energy (SFE) of paramagnetic FeCrCoNiMn High Entropy Alloy (HEA) is investigated as a function of temperature by using *ab initio* calculations based on the exact muffin-tin orbitals method and the coherent potential approximation. We divide the SFE into three major contributions: chemical, magnetic and strain parts. Structural energies, local magnetic moments and elastic moduli are used to estimate the effect of temperature on each term. Calculations show that the SFE of

FeCrCoNiMn HEA is particularly low and has a large positive temperature gradient.

Friday, June 12th, 14:10-14:30

Designing high entropy alloys based on the tabulated physical properties of the constituent elements

• Lajos K. Varga

Wigner Research Center for Physics of Hungarian Academy of Sciences Budapest 1525, POB 49, Hungary

The tabulated physical properties data of the possible constituent elements for high entropy alloys will be revisited. The binary mixing enthalpy, $\Delta H_{\rm mix}$, the atomic radius, r, the valence, z, the electronegativity, χ, the elastic, E, and bulk modulus, B, will be reviewed from different sources and the most appropriate data will be selected and presented for calculating the characteristic quantities for alloy designing:

Mixing enthalpy $$\Delta H_{\rm mix} = \sum_{i=1,j>1}^{n} 4\Delta H_{AB}^{\rm mix} c_i c_j \,,$$

configuration entropy $$\Delta S_{\rm mix} = -R \sum_{i=1}^{n} c_i \ln c_i \,,$$

atomic size mismatch $$\delta r = \sqrt{\sum_{i=1}^{n} c_i \big(1 - r_i / \sum_{i=1}^{n} c_i r_i\big)^2} \,,$$

and electro negativity $$\Delta\chi = \sqrt{\sum_{i=1}^{n} c_i \big(\chi_i - \sum_{i=1}^{n} c_j \chi_j\big)^2} \,.$$

Differences are used for calculating the alloy designing parameters such as: $\Omega = T_m \Delta S_{\rm mix}/|\Delta H_{\rm mix}|$.
New designing parameters will be proposed, such as: $P = \overline{T}_m \Delta S_{\rm mix}/E\delta^2$ and $Q = \Delta H_{\rm mix}/E\delta^2$, where $E = \sum_{i=1}^{n} c_i V_i E_i / \sum_{i=1}^{n} c_i E_i$ and V_i is the molar volume.
Selection rules for solid solution phases in high entropy alloys can be established from diagrams representing Ω, P. and Q versus atomic size mismatch. Electron densities for high entropy alloys obtained by *ab initio* calculations will be compared to those obtained from tabulated data: $n = \sum_{i=1}^{n} c_i z_i / \sum_{i=1}^{n} c_i V_i^a$.
Some diagrams correlating the mechanical properties (hardness and elastic modulus) with electron densities will be presented for bulk amorphous and single-phase high entropy alloys.

Abstracts: Nanostructures

Friday, June 12th, 15:00-15:20

Effect of bottom electrodes on the tunneling electro-resistance in P(VDF-TrFE) based hybrid ferroelectric tunnel junctions for non-volatile memories

• Sayani Majumdar [1] Binbin Chen [1,2] Qin QiHang [1]
Sebastiaan van Dijken [1]

[1] *Nanospin, Department of Applied Physics, Aalto University School of Science, Espoo, Finland*
[2] *National Laboratory of Solid State Microstructures and Department of Physics, Nan-jing University, Nanjing 210093, China*

Manipulation of electronic properties at a single molecular scale by subjecting the molecules to external stimuli like electric or magnetic field holds promises for fascinating science and large range of applications. Recent years have witnessed huge surge in interest for ferroelectric tunnel junctions (FTJ) showing giant tunneling eletroresistance (TER) effect. The FTJs can write and read information using an applied voltage and retain data without any power supply and therefore can be used as non-volatile, energy efficient data storage elements. Here we report a robust, spontaneous, and electrically switchable TER at room temperature in few nano-meter thick, spin-coated films of ferroelectric co-polymer P(VDF-TrFE) (70:30) on different conducting oxide and metallic electrodes. A room temperature conductive-tip atomic force microscopy (AFM), piezo-force microscopy (PFM) and tunneling AFM (TUNA) measurements on the P(VDF-TrFE) thin films on conductive Indium Tin Oxide (ITO), $La_{0.67}Sr_{0.33}MnO_3$ (LSMO), Nb-doped SrTiO3 (Nb-STO) and Au substrates clearly demonstrate that large TER arises due to electrically induced polarization reversal in P(VDF-TrFE) molecules. Time dependent measurements reveal written domains are most stable on the Nb-STO bottom electrodes (Fig. 1) followed by LSMO, ITO and Au bottom electrodes. This finding is of utmost importance for non-volatile hybrid resistive memory elements working under ambient conditions. Also easy, large area and low temperature processing technique of the hybrid devices hold promises for additional advantages of low cost, printable, greener technology solutions for future.

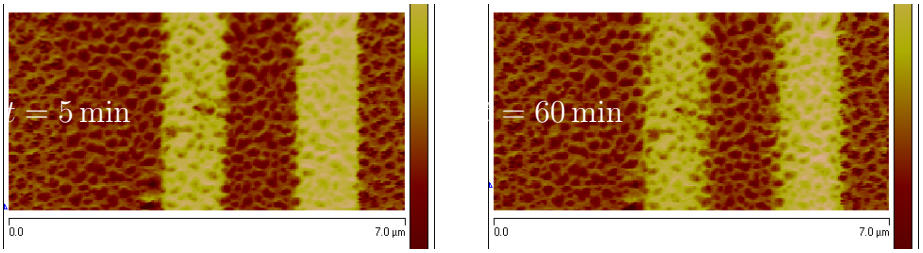


Fig. 1: Kelvin-probe force microscope (KPFM) image of surface potential (left) just after writing and (right) 1 hour after writing on P(VDF-TrFE) films on Nb-STO bottom electrodes showing stable data retention capacity.

Friday, June 12th, 15:20-15:40

Properties of 3*d* transition metal point defects used to stabilize hexagonal $BaTiO_3$ at room temperature

S. K. Nayak [1] H. T. Langhammer [2] W. A. Adeagbo [1]
• W. Hergert [1] T. Müller [2] R. Böttcher [3]

[1] *Martin Luther University Halle-Wittenberg, Institute of Physics, Von-Seckendorff-Platz 1, 06120 Halle, Germany*
[2] *Martin Luther University Halle-Wittenberg, Institute of Chemistry, Kurt-Mothes-Str. 2, 06120 Halle, Germany*
[3] *University of Leipzig, Faculty of Physics and Earth Sciences, Linnéstr. 5, 04103 Leipzig, Germany*

Chromium doped hexagonal barium titanate is studied from first-principles density functional theory using the generalized gradient approximation as the exchange and correlation energy functional. The results are compared with experimental data available from electron paramagnetic resonance (EPR), X-ray diffraction (XRD) and optical absorption spectra and from literature. The probable site for the impurity atom occupancy in the lattice, their probable charge states and the role of oxygen vacancies in their stabilization are investigated. Defect formation energy is used to analyse the role of electronic- and ionic-compensation mechanisms in stabilizing the point defect. Various atomic positions for the oxygen vacancy surrounding the impurity atom are taken into consideration in order to compare with some of the conclusions derived from experiments. Our results on the substitutional site preference and the location of oxygen vacancy in the next-neighbor surrounding of the impurity Cr is in good agreement with experiments.

References

[1] S. K. Nayak *et al.*, Phys. Rev. B **91**, 155105 (2015)

Friday, June 12th, 15:40-16:00

Simulation of nanoindentation of gold nanorods

• Antti Kuronen B. Reischl K. Nordlund

Department of Physics, University of Helsinki, Finland

The atomic force microscope (AFM) can be used to measure mechanical properties

of nanoscale objects, which are too small to be studied using a conventional nanoindenter. The contact mechanics at such small scales, in proximity of free surfaces, deviate substantially from simple continuum models. We present results from atomistic computer simulations of the indentation of gold nanorods using a diamond AFM tip and give insight in the atomic scale processes, involving creation and migration of dislocations, leading to the plastic deformation of the sample under load, and explain the force–distance curves observed for different tip apex radii of curvature, as well as different crystallographic structure and orientation of the gold nanorod samples.

References

[1] B. Reischl, A. Kuronen, and K. Nordlund, Materials Research Express **1**, 045042 (2014)

Friday, June 12th, 16:00-16:20

Defects in Dilute Nitride Solar Cells

• V. Polojärvi [1] A. Aho [1] A. Tukiainen [1] M. Raappana [1] T. Aho [1] A. Schramm [1] M. Guina [1]

[1] *Optoelectronics Research Centre, P.O.B. 692, FIN-33101 Tampere University of Technology, Finland*

Defects in crystal lattice can influence remarkably performance of semiconductor devices. Such parameters as background doping and nonradiative recombination rate are widely caused by defects. High-quality material with low defect densities is in key-role when fabricating high-efficiency multijunction III-V semiconductor solar cells. GaInNAs(Sb) is a promising material for high-efficiency multijunction solar cells. Well over 40 % conversion efficiencies have been demonstrated from molecular-beam-epitaxy grown three-junction solar cell with GaInNAsSb bottom junction [1]. However, relatively low growth temperatures and incorporation of N induces defects to the material, reducing its current and voltage generation [2]. Therefore, detailed knowledge about defects and their formation is essential when fabricating high-quality GaInNAs(Sb). We used capacitance spectroscopy to characterize defects in dilute nitride and antimonide materials. Defects and their influence on solar cell operation are discussed.

References

[1] Allen *et al.*, 9th International Conference on Concentrator Photovoltaic Systems , Japan (2013)

[2] A. Aho *et al.*, Solar Energy Mater. Solar Cells **124**, 150-158 (2014)

List of participants

Adeagbo, Waheed, (Talk, p. 16)
Martin Luther University Halle-Wittenberg, Germany
Email: waheed.adeagbo@physik.uni-halle.de

Chichova, Dina
University of Turku, Finland
Email: dinachichova@gmail.com

Dahl, Johnny
University of Turku, Finland
Email: jpvdahl@gmail.com

Dong, Zhihua, (Talk, p. 14)
Royal Institute of Technology, Stockholm, Sweden
Email: yndldong@163.com

Elovaara, Tomi, (Talk, p. 19)
University of Turku, Finland
Email: tkelov@utu.fi

Fazakas, Eva
Wigner Research Center for Physics, Budapest, Hungary
Email: fazakas.eva@wigner.mta.hu

Geilhufe, Matthias, (Talk, p. 8)
Martin Luther University Halle-Wittenberg, Germany
Email: geilhufe@mpi-halle.mpg.de

Gloos, Kurt, (Talk, p. 13)
University of Turku, Finland
Email: kurt.gloos@utu.fi

Granroth, Sari, (Talk, p. 20)
University of Turku, Finland
Email: sasuma@utu.fi

Huang, Shuo, (Talk, p. 30)
Royal Institute of Technology, Stockholm, Sweden
Email: shuoh@kth.se

Kim, Dongyoo, (Talk, p. 12)
Royal Institute of Technology, Stockholm, Sweden
Email: kdyoo999@gmail.com

Kuronen, Antti, (Talk, p. 35)
University of Helsinki, Finland
Email: antti.kuronen@helsinki.fi

Laukkanen, Pekka
University of Turku, Finland
Email: pekka.laukkanen@utu.fi

Lehmusto, Juho
Abo Akademi University, Finland
Email: juho.lehmusto@abo.fi

Li, Ruihuan, (Talk, p. 28)
Royal Institute of Technology, Stockholm, Sweden
Email: ruihuan@kth.se

Li, Wei
Royal Institute of Technology, Stockholm, Sweden
Email: wei2@kth.se

Li, Xiaoqing, (Talk, p. 30)
Royal Institute of Technology, Stockholm, Sweden
Email: xiaoqli@kth.se

Lu, Song, (Talk, p. 22)
Royal Institute of Technology, Stockholm, Sweden
Email: songlu@mse.kth.se

Majumdar, Sayani, (Talk, p. 34)
Aalto University, Espoo, Finland
Email: sayani.majumdar@aalto.fi

Malmivirta, Mika
University of Turku, Finland
Email: mika.malmivirta@utu.fi

Marmodoro, Alberto, (Talk, p. 9)
Max Planck Institute of Microstructure Physics, Halle, Germany
Email: a.marmodoro@googlemail.com

Nagy, Agnes, (Talk, p. 8)
University of Debrecen, Hungary
Email: anagy@phys.unideb.hu

Nayak, Sanjeev Kumar, (Talk, p. 17)
Martin Luther University Halle-Wittenberg, Germany
Email: sanjeev.nayak@physik.uni-halle.de

Nurmi, Eero
University of Turku, Finland
Email: eknurm@utu.fi

Östlin, Andreas, (Talk, p. 12)
Royal Institute of Technology, Stockholm, Sweden
Email: andreas.kth@gmail.com

Paturi, Petriina
University of Turku, Finland
Email: petriina.paturi@utu.fi

Polojärvi, Ville, (Talk, p. 36)
Tampere University of Technology,Finland
Email: ville.polojarvi@tut.fi

Punkkinen, Marko
University of Turku, Finland
Email: marko.punkkinen@utu.fi

Ropo, Matti
Tampere University of Technology,Finland
Email: matti.ropo@tut.fi

Schönecker, Stephan, (Talk, p. 22)
Royal Institute of Technology, Stockholm, Sweden
Email: stesch@kth.se

Tian, Li-Yun, (Talk, p. 23)
Royal Institute of Technology, Stockholm, Sweden
Email: liyunt@kth.se

Varga, Lajos, (Talk, p. 31)
Wigner Research Center for Physics, Budapest, Hungary
Email: varga.lajos@wigner.mta.hu

Wang, Guisheng, (Talk, p. 27)
Royal Institute of Technology, Stockholm, Sweden
Email: guisheng@kth.se

Organization committee

Scientific and General Organization:

Hergert, Wolfram, (Talk, p. 35)
Martin Luther University Halle-Wittenberg, Germany
Email: wolfram.hergert@physik.uni-halle.de

Hoffmann, Martin, (Talk, p. 18)
Martin Luther University Halle-Wittenberg, Germany
Email: hoffmann@mpi-halle.de

Kokko, Kalevi
University of Turku, Finland
Email: kokko@utu.fi

Lahti, Antti
University of Turku, Finland
Email: ailaht@utu.fi

Levämäki, Henrik, (Talk, p. 26)
University of Turku, Finland
Email: hpleva@utu.fi

Vitos, Levente
Royal Institute of Technology, Stockholm, Sweden
Email: levente.vitos@fysik.uu.se

Notes