MM 3: Computational Materials Modelling I

Time: Monday 11:00–13:00 Location: IFW B

MM 3.1 Mon 11:00 IFW B

Properties of positrons at defects in metal — •Martin Offenberger[1], Hubert Ebert[1], and John Banhart[2] — [1]Ludwig-Maximilians-Universität München — [2]Helmholtz Zentrum Berlin

Positron annihilation is a well established tool to study defects in metals in experiment. To simulate positron annihilation experiments, an accurate and efficient description of both positrons and defects is needed. To calculate clusters of impurity atoms in a metal host, we use the Korringa-Kohn-Rostoker Green's function method (KKR-GF). This approach deals with the defect region by means of the Dyson equation instead of a supercell approach, avoiding artificial boundary conditions. Positrons are then calculated according to the conventional scheme suggested e.g. by Boroński and Nieminen. Results of our calculations presented include positron charge distributions, density of states and annihilation lifetimes for a variety of defects in Aluminium. In addition, the properties of defects like vacancies and transition metal impurity-vacancy dimers as positron traps will be discussed.

MM 3.2 Mon 11:15 IFW B

Ab-initio-based prediction of the vacancy concentration in the $Ni_{<50}Al_{50}$ B2 phase — •Tobias C. Kerscher[1], Daniel Lerch[2], Gus L. W. Hart[3], Quinn O. Snell[4], and Stefan Müller[1] — [1]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, 21073 Hamburg, Germany — [2]Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik 2, Staudtstr. 7, 91058 Erlangen, Germany — [3]Brigham Young University, Department of Physics and Astronomy, Provo UT 84602, USA — [4]Brigham Young University, Computer Science Department, Provo UT 84602, USA

The B2 phase of Ni–Al gains its technical importance from the high melting point (1638 °C). Off its ideal 50-50 stoichiometry, this B2 phase is stabilised by the formation of vacancies on the Ni sublattice. We use our code UNCLE [1] to construct an ab-initio-based cluster-expansion Hamiltonian for this ternary (Ni, Al, vacancy) system. Thermodynamic Monte Carlo simulations in the (quasi)grand-canonical ensemble are applied to account for configurational entropy and to predict the equilibrium concentration of the vacancies as a function of temperature. Since point defect concentrations are expected to be in the order of ppm, the correspondingly large Monte Carlo cells are addressed with the help of a recently demonstrated parallel Monte Carlo implementation in UNCLE.

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[1] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003.

MM 3.3 Mon 11:30 IFW B

Ab initio determination of diffusion mechanisms in FeAl — •Niko Sandschneider, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

Iron aluminides are a promising material class for industrial high temperature applications. FeAl shows a very high vacancy concentration (several percent at T>1000 K) which severely affects its mechanical properties. It is therefore crucial to understand the generation and diffusion behavior of those vacancies.

The simplest diffusion mechanism which preserves long-range order in B2-FeAl is the next-nearest neighbor (NNN) jump of a vacancy. As a first step we performed ab initio calculations to determine the formation energies of the defects in FeAl. Four defects were investigated, namely vacancies and antisite atoms on the Fe and Al sublattices. We found that the Al vacancy has a large formation energy compared to the other defects. Therefore the NNN jump was only investigated for Fe vacancies. In a second step we calculated the migration barrier of this process using the climbing image nudged elastic band method.

Several more sophisticated mechanisms are proposed in the literature. A very promising candidate is the triple defect mechanism. We also performed nudged elastic band calculations for this mechanism and found a migration barrier which is significantly lower than for the NNN jump and several other diffusion mechanisms. We therefore conclude that the triple defect mechanism is the energetically most favorable diffusion mechanism.

MM 3.4 Mon 11:45 IFW B

Ab-initio and atomistic study of the ferroelectric properties of Cu doped potassium niobate — •Sabine Körbel and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

$KNbO_3$ is one end member of the solid solution $(K, Na)NbO_3$ (KNN), which has promising ferroelectric properties to become a future lead-free substitute for lead zirconate titanate $Pb(Zr, Ti)O_3$ (PZT) in piezoelectric actors and sensors. Both KNN and PZT exhibit a phase transition with composition and a morphotropic phase boundary, at which enhanced piezoelectric coefficients are obtained. The material properties of PZT and KNN are commonly optimized by doping. E.g., CuO can be added when fabricating KNN as a sintering aid. Ab initio density functional theory and atomistic simulation using a classical shell model potential have been combined to investigate low Cu concentrations in the $KNbO_3 - CuNbO_3$ system. The atomistic model predicts a morphotropic phase boundary at a few percent Cu, analoguous to the one found in the $LiNbO_3 - KNbO_3$ system [1,2].

[1] Y. Guo, K. Kakimoto, and H. Ohsato, Appl. Phys. Lett. **85**, 4121 (2004).
[2] D. I. Bilc and D. J. Singh, Phys. Rev. Lett. **96**, 147602 (2006).

MM 3.5 Mon 12:00 IFW B

Defects in ferrite: from quantum-mechanical calculations to long-range elastic effects — •Alexander Udyansky[1], Johann von Pezold[1], Alexey Dick[1], Vladimir Bugaev[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Interstitial Fe-based solid solutions with a low content of C, N, O, B, C+N and H impurities have been studied by combining first principles simulations with the reciprocal space microscopic elasticity theory (MET). This approach allows for a highly efficient description of long-range elastic interactions, which generally control interstitial-interstitial interactions. The short-range chemical interactions, as well as the parameters entering the MET are obtained by density functional theory (DFT) in the generalized gradient approximation, using rather modest supercell sizes. The proposed approach provides a direct insight into the formation mechanism of martensite and its stability limit. For example, tetragonal states are predicted to be preferred even at low impurity concentrations due to a thermodynamically driven orientational ordering of impurities. Furthermore we were able to predict the low impurity concentration part of Fe-based solid solutions phase diagrams and its dependence on the local strain state of the system. Finally, the impurity content is found to strongly affect the vacancy concentration within the host matrix.

MM 3.6 Mon 12:15 IFW B

Ab initio study of effect of non-magnetic impurities on the structure and properties of grain boundaries and free surfaces in nickel — •Monika Všianská[1,2] and Mojmír Šob[1,2] — [1]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [2]Istitute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

We have studied segregation of sp-elements of the 3rd, 4th and 5th period (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at the Σ5(210) grain boundary (GB) and (210) free surface (FS) in fcc nickel. We analysed the geometric configuration and the distribution of magnetic moments at the GB and FS without and with impurities. Whereas there is a slight enhancement of magnetization at the clean GB with respect to bulk nickel, the studied impurities entirely kill or strongly reduce ferromagnetism at the GB and its neighbourhood. We also determined the embrittling energy and its chemical and mechanical part from the difference between the GB and FS binding energies on the basis of the Rice-Wang model. We predict interstitially segregated Si as a GB cohesion enhancer, substitutionally segregated Al and interstitially segregated P with none or minimal strengthening effect and interstitially segregated S, Ge, As, Se and substitutionally segregated Ga, In, Sn, Sb and Te as GB embrittlers in Ni.

MM 3.7 Mon 12:30 IFW B

Ab initio study of energetics and magnetism of Fe, Co and Ni along the trigonal deformation path — Martin Zelený[1], Martin Friák[2,3], and •Mojmir Šob[4,1] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Max-Planck Institut für Eisenforschung, GmbH, Düsseldorf, Germany — [3]Institute of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have calculated total energies of iron, cobalt and nickel in several magnetic phases as a function of atomic volume and trigonal deformation and found the phase boundaries between various magnetic modifications in Fe and Ni. In case of Ni, these phase boundaries occur even at the experimental atomic volume. On the other hand, Co keeps its ferromagnetic order in the whole region of the volume and shape deformation studied. Fe does not exhibit any transition between the ferromagnetic and non-magnetic arrangement, but at low atomic volumes around the fcc structure, phase boundaries between the ferromagnetic high-spin, ferromagnetic low-spin and antiferromagnetic states have been found.

MM 3.8 Mon 12:45 IFW B

Point-defect-mediated dehydrogenation of alane — •Lars Ismer, Anderson Janotti, and Chris G Van de Walle — University of California at Santa Barbara, CA 93106, United States

For the engineering of better hydrogen storage materials a systematic understanding of their hydrogen sorption kinetics is crucial. We present a systematic analysis of the dehydrogenation kinetics of alane (AlH3), one of the prime candidate materials for hydrogen storage. Using hybrid-density functional calculations we determine the concentrations and mobilities of point defects and their complexes. Kinetic Monte Carlo simulations are used to describe the full dehydrogenation reaction. We show that under dehydrogenation conditions charged hydrogen vacancy defects form in the crystal, which have a strong tendency towards clustering. The vacancy clusters denote local nuclei of Al phase, and the growth of these nuclei eventually drives the AlH3/Al transformation. However, the low concentration of vacancy defects limits the transport of hydrogen across the bulk, and hence acts as the rate-limiting part of the process. The dehydrogenation is therefore essentially inactive at room temperature, explaining why AlH3 is metastable for years, even though it is thermodynamically unstable. Our derived activation energy and dehydrogenation curves are in excellent agreement with the experimental data, providing evidence for the relevance of bulk point-defect kinetics. Based on our results we argue that manipulating vacancy defect concentrations, e.g., by the usage of irradiation, will allow control over hydrogen sorption kinetics, opening up new engineering strategies.