MM 27: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Alloys and Mechanical Response

Time: Wednesday 15:00–18:15 Location: H44

MM 27.1 Wed 15:00 H44

Phase stability and disorder in ThMn12 type ferromagnetic intermetallics — •Anna J. Lehner[1,2], Daniel F. Urban[2], and Christian Elsässer[2] — [1]IAM-CMS, KIT, Karlsruhe, Germany — [2]Fraunhofer IWM, Freiburg, Germany

Rare earth (RE) and transition metal (TM) intermetallics of the $ThMn_{12}$-structure type ('1-12') are widely discussed as good candidates in the search for new hard magnetic materials with considerably less RE-content than state-of-the-art $Nd_2Fe_{14}B$ or $SmCo_5$ magnets. Some binary RE-Fe phases with $ThMn_{12}$ structure, namely the most promising $NdFe_{12}$, are experimentally stable only as thin films. By addition of alloying elements (e.g. Ti) stable ternary bulk crystals with the $ThMn_{12}$ structure can be obtained experimentally and serve for validation of promising intrinsic magnetic properties which have been predicted by a screening using density functional theory [1]. In addition to magnetic properties, predicting thermodynamic phase stabilities extends the value of the computational screening. In this study we focus on the effects of configurational disorder on the thermodynamic phase stability. We combine combinatorial first-principles total energy calculations with a cluster expansion (CE) for the configurational energy associated with TM site disorder. We relate the basis functions of the CE to the structural motives in the topologically closed packed (tcp) 1-12 phase and discuss the transferability of our model to other tcp phases. Finally, the robustness of the CE-model for substituents of varying atomic radius (Co,Si,Ti) is critically assessed. [1] W. Körner, G. Krugel, and C. Elsässer, Sci. Rep. 6, 24686 (2016).

MM 27.2 Wed 15:15 H44

Ab initio study of plastic deformation in Fe_2Nb Laves phase — •Alvin Noe Ladines[1], Thomas Hammerschmidt[1], Ali Zendegani[2], Tilmann Hickel[2], Ralf Drautz[1], and Joerg Neugebauer[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]Max Planck Institute for Iron Research, Düsseldorf, Germany

The Fe_2Nb Laves phase is technologically relevant for strengthening advanced stainless steels. An atomistic understanding of the mechanisms of plastic deformation of this phase is lacking. We use density functional theory (DFT) to calculate the generalized stacking faults for various deformation modes. Our calculations reveal that synchroshear is the most energetically favorable deformation mechanism for the C14-Fe_2Nb Laves phase. We further study the influence of intrinsic point defects and alloying elements Al, Si, Cr, Ni, Mo and Zr on the energy of the stacking faults. Vacancies tend to lower the energy barrier for synchroshear deformation, while anti-site defects do not have a systematic effect on stacking fault energies. The alloying elements are shown to soften the C14-Fe_2Nb Laves phase.

MM 27.3 Wed 15:30 H44

Understanding the thermodynamics and kinetics of precipitate formation in Al-Sc-Zr alloys — •Ankit Gupta[1], Yulia Buranova[2], Vladislav Kulitcki[2], K. Li[3], Yong Du[3], Biswanath Dutta[1], Tilmann Hickel[1], Jörg Neugebauer[1], Gerhard Wilde[2], and Sergiy V. Divinski[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Institute of Materials Physics, University of Münster, Germany — [3]Institute for Materials Microstructure, Central South University, Changsha, China

The thermal stability of Al-based alloys is enhanced typically by improving the coarsening resistance of second phase particles. A classic example is the addition of Zr to Al-Sc alloys where the Zr segregation at particle-matrix interfaces thermally stabilizes the Al_3Sc particles. Our experiments performed under varying processing conditions result in a rich microstructure characterized predominantly by two types of second phase $Al_3(Sc,Zr)$ particles: one with uniform distribution of Sc and Zr and the other with a Sc-rich core and Zr-rich shell. The chemically heterogeneous core-shell structure exhibits an anisotropic Zr distribution along different orientations of precipitate interfaces. Using DFT based calculations, we quantify this sensitive interplay between the bulk and interfacial thermodynamics causing the observed two-phase microstructure. The computed mixing enthalpy trends predict homogeneously distributed Sc and Zr on the Sc-sublattice to be the thermodynamically stable configuration. The relevance of interfacial segregation and solute interactions in explaining the chemical anisotropy and the subsequent growth of core-shell structures are shown.

MM 27.4 Wed 15:45 H44

Multi-Scale Modelling of Guinier-Preston Zone Formation in Al-Cu Alloys — •Tobias Stegmüller and Ferdinand Haider — University of Augsburg, Institute for Physics, Chair for Experimental Physics I, 86135 Augsburg, Germany

The investigation of precipitation processes in modern aluminium alloys plays an important role for the design of many material properties like strength or corrosion resistance. The influence of ageing time and temperature constitute the key for a quantitative understanding of precipitate formation.

The prediction of the evolution of the precipitate size distribution is a powerful tool for the characterisation of an alloy temper state. In this work a multi-scale approach, covering nucleation, growth and coarsening of early stage precipitates in binary Al-Cu alloys, the Guinier-Preston zones (GPZ), will be presented. Starting from DFT calculations and Cluster Expansion construction, followed by Monte Carlo free energy calculations, a meso-scale Cluster Dynamics model is constructed. By following this approach, the model is able to predict the evolution of size distributions of GPZ for different alloy compositions and ageing temperatures.

To validate the model, kinetic Monte Carlo simulations on the precipitation of GPZ were performed and the results for the evolution of average precipitate size, precipitated fraction of solute and the number density of precipitates agree well with the results obtained by Cluster Dynamics. The formulation of the multi-scale approach, its results and the comparison to the Monte Carlo simulations will be presented.

MM 27.5 Wed 16:00 H44

mergence of complex patterns in CoTixZr1-xSb1-ySny and NiTixZr1-xSb1-ySny half-Heuslers — •Joaquin Miranda Mena and Thomas Gruhn — Biomaterials, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany

We present the effects of the chemical substitution on the phase separation of alloyed half-Heuslers with formula $CoTi_xZr_{1-x}Sb1-ySn_y$ and $NiTi_xZr_{1-x}Sb_{1-y}Sn_y$ over a wide range of x and y concentrations. The combination of different length-scales methods -Density Functional Theory, Monte Carlo simulations and Mean field calculations- allows us to predict macroscopic properties which are relevant for the material production. We found that complex textures composed of different phases emerge for certain concentrations as the temperature is lowering. These textures could open a new strategy to reduce the heat conductivity which is hampering the performance of half-Heuslers as good thermoelectrics.

MM 27.6 Wed 16:15 H44

First principle studies of Electronic, Magnetic, and mechanical properties of (Pt and Ru) ZrTiAl Quaternary Heusler Alloy — •Ramesh Paudel[1] and Jingchuan Zhu[1,2] — [1]School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China — [2]2.*National Key Laboratory of Science and Technology on Advanced in Special Environments, Harbin Institute of Technology, Harbin 150001, China

In this study, we investigated the structural, magnetic, mechanical properties of (Pt and Ru) ZrTiAl quaternary Heusler alloys by utilizing density functional theory within the CASTEP code. Investigated equilibrium lattice parameters of these compounds are in great concurrence with other theoretical work. The total magnetic moments of (PT and Ru) ZrTiAl were obtained to be 3*B and 2.99*B per unit formula respectively obeys the Slater Pauling rule. (PT and Ru) ZrTiAl is found to have a spin-flip/half-metallic gap in the minority spin channel while the majority spin channel is metallic. Therefore, both composites showed half-metallic nature and 100 percent spin polarization at the Fermi level. The calculated mechanical results revealed that both materials are mechanically steady and ductile nature. The RuZrTiAl alloy is predicted for the very first time by utilizing the GGA scheme. Our investigated results could be worthwhile for future experimental work and application for spintronic devices.

15 min. break

MM 27.7 Wed 16:45 H44

Numerical simulation of deformation of aluminum alloy during novel Conform-HPTE process — •Jiamin Hu[1,2], Roman Kulagin[2], Yulia Ivanisenko[2], and Hui Zhang[1] — [1]College of Materials Science and Engineering, Hunan University, Changsha 410082, China — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe 76021, Germany

In this paper, we explored the feasibility of a new continuous severe plastic deformation (SPD) technique, which combines continuous extrusion forming (Conform) and high pressure torsion extrusion (HPTE), we defined it as Conform-HPTE. A finite element method (FEM) simulation model of this process was established using QForm software. The results showed that the novel Conform-HPTE technique can owe both the advantages of Conform and HPTE, thus it could be used for industrial production of aluminum alloys due to its low energy input, no limit for billet length and large shear strain during one deformation pass. The effects of tool geometry and processing parameters on the extrusion load, temperature, strain evolution and metal flow during the Conform-HPTE process were discussed.

MM 27.8 Wed 17:00 H44

Hydrogen enhanced cross-slip of dislocations in the vicinity of grain boundaries in nickel — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Extensive experimental observations indicate the presence of nanovoids and an increase of the free volume along grain boundaries in hydrogen contaminated metals. This phenomenon is rate-dependent and assumed to be connected to hydrogen embrittlement of Ni based alloys. However, an understanding of the underlying mechanism is lacking. In the present study a mechanism for an enhanced cross slip of the dislocations in the close vicinity of the grain boundaries is demonstrated by performing molecular dynamics (MD) simulations. The interaction of the screw dislocations with a variety of symmetric tilt grain boundaries in H-charged and H-free bicrystalline nickel specimens are examined. The presence of the segregated hydrogen atoms at the grain boundaries induces a stress field around them and thus the barrier for cross-slip of screw dislocations considerably decreases. The enhanced cross slip of dislocations facilitates the formation of jogs *below a critical loading rate *. These jogs are found to emit vacancies during glide processes. The mechanism discovered in this study shows nano-scale evidence of a rate sensitive enhanced vacancy formation and a subsequent increase in the free volume along the grain boundaries in the presence of H.

MM 27.9 Wed 17:15 H44

Electronic structure and lithium storage mechanism of high-rate niobium oxide-based crystallographic shear phases from first principles — •Can P. Koçer[1], Kent J. Griffith[2,3], Clare P. Grey[3], and Andrew J. Morris[4] — [1]Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge — [2]Department of Materials Science and Engineering, Northwestern University — [3]Department of Chemistry, University of Cambridge — [4]School of Metallurgy and Materials, University of Birmingham

Crystallographic shear phases of niobium oxide have shown unprecedented high-rate performance as high-voltage anodes for lithium ion batteries [1,2]. The electronic structure, lithium insertion mechanism, and lithium dynamics of these compounds remain relatively unexplored, largely due to their novelty and complexity. In this talk, I will present recent work by our group on the electronic structure and lithium insertion mechanism of crystallographic shear phases in the Wadsley-Roth family, including mixed-metal TiO_2-Nb_2O_5, and WO_3-Nb_2O_5 phases. Our work has explored interesting electron localisation-delocalisation transitions on n-type doping in the niobium suboxides [3], and provides a unified mechanistic picture for the structural changes in the entire family of crystallographic shear phases [4]. I will discuss challenges associated with modelling these materials, and will point out future directions for experimental and first-principles studies.

[1] K. J. Griffith et al., Nature **559**, 556-563 (2018) [2] K. J. Griffith et al., Journal of the American Chemical Society **138**, 8888 (2016) [3] C. P. Koçer et al. (*in preparation*) [4] C. P. Koçer et al. (*in preparation*)

MM 27.10 Wed 17:30 H44

Effect of strain on ionic conductivity of cubic Li6.25Al0.25La3Zr2O12 solid electrolyte — •Ashkan Moradabadi[1,2] and Payam Kaghazchi[3] — [1]Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin Takustr. 3, 14195, Berlin — [2]FG Materialmodellierung, Technische Universität Darmstadt, Otto-Berndt-Str. 3 64287 Darmstadt — [3]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research, IEK-1, D-52425 Jülich, Germany

Al-doped cubic-Li7La3Zr2O12 (Al-LLZO) is a promising solid electrolyte material for all-solid-state batteries (ASSBs). However, Al-LLZO shows a poor performance in practice mainly due to a high resistance, particularly at the electrolyte/electrode interfaces. Interfacial and lattice mismatch induced strain is a key factor in controlling the rate performance of ASSBs. In this presentation, I will discuss the influence of strain on the mechanism and conductivity of Li ion transport in Al-LLZO using DFT-based thermodynamics of defects and ab initio molecular dynamics. Our calculations on the formation energy (concentration of carriers) and migration barrier (mobility of carriers) of ions in Al-LLZO will be presented. Furthermore, by comparing PBE and HSE06 results, the effect of XC correlation functional on the stability and defect chemistry of Al-LLZO will be discussed. The results of this work can be an important step toward understanding the effect of strain on the rate capability of ASSBs.

MM 27.11 Wed 17:45 H44

Ab initio study of tetragonal and trigonal bcc-fcc transformations in Ti-Al-Mo system — •Neda Abdoshahi[1], David Holec[1], Martin Friák[2], and Mojmir Šob[2] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic

Motivated by a recently reported martensitic transformation in the Ti-Al-Mo intermetallic system, we employed first principles calculations to study this process on an atomic level. Our calculations reveal a spontaneous transformation from the unstable β o (bcc ordered) to the stable γ phase: there is no energy barrier along the transformation path, and an overall energy difference is *140 meV/at. for β o * γ. It is further shown that a chemical disorder reduces the driving force (total energy difference) for the β * γ dis transformation to essentially "zero" and introduces a small energy barrier of about 10 meV/at..

Next we have investigated a trigonal transformation path, connecting bcc, simple cubic (sc) and fcc structures. Not only it yields a high energy barrier of * 890 meV/at. for β 0 * γ * transformation, but it also leads to another fcc-based ordered binary compound, namely the L1 2 structure (γ *) instead of the true TiAl L1 0 (γ) ground state. Consequently we exclude the trigonal transformation path for the MTs in TiAl. In the final part we explore the impact of Mo on the stabilization of the β/β o TiAl with respect to the γ phase.

MM 27.12 Wed 18:00 H44

An *ab initio* perspective on reversible martensitic transformations in Ti-Ta shape memory alloys — •Alberto Ferrari[1], Davide G. Sangiovanni[1,2], Jutta Rogal[1], and Ralf Drautz[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183 Linköping, Sweden

Shape memory alloys exhibit reversible martensitic transformations (MTs) when temperature or stresses are applied. Modelling these transformations from first principles is not trivial, since static calculations are usually not sufficient to explore the most important aspects of the MTs, such as the Ehrenfest order of the phase transitions, the range of stability of the low- and high-temperature phases, and their free energy barrier. In this contribution, a fully *ab initio* strategy to characterize MTs in alloys is presented. The temperature dependent order parameters of a MT are calculated with *ab initio* molecular dynamics; then, the free energy of the MT, from which all the relevant thermodynamic properties of the MT can be derived, is modelled with a Landau polynomial expansion. The parameters of this expansion are completely extracted from first principles. This approach is applied to the high-temperature shape memory alloy Ti-Ta, for which very small values for the free energy barrier and the region of metastability are observed.