

## MM 6: Computational Materials Modelling: Defects / Alloys

Time: Monday 15:45–18:30

Location: H44

MM 6.1 Mon 15:45 H44

**Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases** — •ZHUOCHENG XIE<sup>1</sup>, DIMITRI CHAURAUD<sup>2,3</sup>, ACHRAF ATILA<sup>2,3</sup>, ERIK BITZEK<sup>2,3</sup>, SANDRA KORTEKERZEL<sup>1</sup>, and JULIEN GUÉNOLÉ<sup>4</sup> — <sup>1</sup>Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — <sup>3</sup>Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — <sup>4</sup>Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, 57070 Metz, France

In Laves phases, synchroshear is the dominant basal slip mechanism. It is accomplished by the glide of synchro-Shockley dislocations. However, the atomic-scale mechanisms of motion of such zonal dislocations are still not well understood. In this work, using atomistic simulations, two 30° synchro-Shockley dislocations with different Burgers vectors and core structures and energies are identified. We demonstrate that nucleation and propagation of kink pairs is the energetically favorable mechanism for the motion of the synchro-Shockley dislocation. Vacancy hopping and interstitial shuffling are identified as two key mechanisms related to kink propagation and we investigated how vacancies and antisite defects assist kink nucleation and propagation, which is crucial for kink mobility. These findings provide insights into the dependency on temperature and chemical composition of plastic deformation induced by zonal dislocations in topologically close-packed phases.

MM 6.2 Mon 16:00 H44

**Macroscopic characteristics of plastic deformation described through dislocation mobility properties** — •SERGEI STARIKOV, ANTOINE KRAYCH, and MATOUS MROVEC — Ruhr University Bochum, ICAMS, Germany

Plastic deformation of bcc metals is a complicated phenomenon that links a behaviour of crystal defects with the macroscopic change of a sample shape. It is known that one of the basic mechanisms of plasticity is a motion of dislocations under applied stress. In this work, on the example of Mo and Nb, the study of plastic deformation in bcc metals was carried out with large-scale atomistic modelling. The temperature-dependent mobility functions of screw and edge dislocations were calculated from molecular dynamics simulation. The simulations of screw dislocation movement under applied shear stress revealed that the process can proceed in two different regimes: through thermally activated motion and athermal motion. Hence, the dislocation velocity depends on the shear stress in a non-trivial way. The calculated data provide a way to evaluate the basic macroscopic characteristics of plastic deformation at various temperatures and strain rates.

MM 6.3 Mon 16:15 H44

**Analytic description of grain boundary segregation, tension, and formation energy in the copper–nickel system** — TAMARA KRAUSS, FELIX FISCHER, and •SEBASTIAN EICH — Institut für Materialwissenschaft — Lehrstuhl für Materialphysik, Universität Stuttgart

In this atomistic study, a recently proposed segregation model [1] is applied to segregation data of an exemplary  $\Sigma 5$  grain boundary (GB), which is investigated using a copper–nickel embedded-atom method potential. Segregation in the semi-grandcanonical ensemble is systematically studied by varying the chemical potential in order to explore the full composition range for temperatures from 500 K to 1000 K. As a major thermodynamic feature, the mentioned segregation model avoids the usage of *interface compositions*, for which an arbitrary volume must be defined, but rather models the thermodynamically unambiguous solute excess. It was shown that the solute excess and the interface formation energy could be described very accurately over a wide range of temperatures and over the entire composition. Since the model was initially derived for systems without lattice mismatch, the copper–nickel system with a mismatch of roughly 2.7% is chosen in this study to further extend the segregation model by a linear-elastic theory to also account for the interface tensions. Using this extended model, it will be shown that the solute excess, GB tensions, and GB formation energies can be derived from an effective energy of segregation for all temperatures and over the whole composition range [2].

- [1] T. Krauß, S. M. Eich, Acta Mater. 187, 73 (2020)  
[2] F. Fischer, S. M. Eich, Acta Mater. 201, 364 (2020)

MM 6.4 Mon 16:30 H44

**Impurity segregation at grain boundaries in bcc iron: large scale models based on machine learned interatomic potentials** — •PETR ŠESTÁK<sup>1</sup>, MONIKA VŠIANSKÁ<sup>1,2</sup>, PAVEL LEJČEK<sup>1,3</sup>, and MIROSLAV ČERNÝ<sup>1</sup> — <sup>1</sup>Central European Institute of Technology, CEITEC BUT, Brno University of Technology, Purkyňova 123, CZ-616 69 Brno, Czech Republic — <sup>2</sup>Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37 Brno, Czech Republic — <sup>3</sup>Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, CZ-182 21 Prague 8, Czech Republic

In this work, we employed on the fly machine learning (ML) as it is implemented in the current version of the VASP to study segregation of Sn, P and Ge atoms at selected GBs (e.g.  $\Sigma 3(112)$ ,  $\Sigma 3(111)$ ,  $\Sigma 5(310)$ ,  $\Sigma 5(210)$ ,  $\Sigma 13(510)$ ,  $\Sigma 13(320)$ , etc.) in bcc iron. Segregation energies were obtained using small supercells (<100 atoms), medium cells (~400 atoms) and also larger cells (>1000 atoms). Data obtained from the small and medium cells were compared with results of ab initio calculations as well as with available experimental data and predictions. This comparison serves as a benchmark of the interatomic potentials received from ML. The comparison shows that the segregation energies and some other GBs characteristics obtained for small cells are very consistent with ab initio simulations which bring a proof of reliability of interatomic potentials. The obtained results revealed that using small simulation cells (leading to high concentrations of impurity atoms), typical for ab initio simulations, might not be sufficient to predict correct segregation energies.

MM 6.5 Mon 16:45 H44

**An efficient method to access the grain boundary parameter space with atomistic simulations** — •TIMO SCHMALOFSKI<sup>1</sup>, MARTIN KROLL<sup>2</sup>, REBECCA JANISCH<sup>1</sup>, and HOLGER DETTE<sup>2</sup> — <sup>1</sup>ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany — <sup>2</sup>Department of Mathematics, Ruhr-University Bochum, 44780 Bochum, Germany

A grain boundary (GB) is a two dimensional defect in solids with significant influence on different material properties. It describes the interface between two grains with different orientations and is thus defined by five macroscopic degrees of freedom (DOF), 2 from the rotation axis, 1 from the misorientation angle and 2 from the grain boundary normal vector. The GB energy as a function of the DOF can be obtained e.g. by atomistic simulations. However, a systematic sampling of the 5D grain boundary parameter space, or even lower-dimensional subspaces of it, comes with several challenges. To overcome them, a sampling method is needed, which only needs a small number of data points and can automatically find the cusps (deep minima) in the energy while sampling. Recently we introduced a sequential sampling technique which fulfills both [1] in the 1D subspace of symmetrical tilt grain boundaries. Now this sequential sampling technique will be evaluated for a 2D analysis of the energy as a function of GB plane inclination for fixed misorientations. [1] Kroll, M., Schmalofski, T., Dette, H. and Janisch, R. (2022), Efficient Prediction of Grain Boundary Energies from Atomistic Simulations via Sequential Design. Adv. Theory Simul. 2100615.

## 15 min. break

MM 6.6 Mon 17:15 H44

**Electronic band gap of  $\text{Al}_x\text{Sc}_{1-x}\text{N}$ : a comparison of CPA and SQS** — •JAN M. WAACK<sup>1,2</sup>, MARKUS KREMER<sup>1,2</sup>, MICHAEL CZERNER<sup>1,2</sup>, and CHRISTIAN HEILIGER<sup>1,2</sup> — <sup>1</sup>Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — <sup>2</sup>Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Calculating physical properties of random substitutional solid solutions such as  $\text{Al}_x\text{Sc}_{1-x}\text{N}$  requires specific methods such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2]. We compare the CPA in the framework of the atomic sphere approximation (ASA) Korringa-Kohn-Rostoker (KKR) density functional theory (DFT) with the SQS using the plane-wave pseudopotential DFT to calculate the lattice parameters and electronic band struc-

tures of the face-centered cubic phase of  $\text{Al}_x\text{Sc}_{1-x}\text{N}$  (with  $0 \leq x \leq 1$ ).

Using the low-computational-cost LDA-1/2 quasiparticle method[3] to calculate the electronic band structures within SQS and CPA, we present the first implementation of LDA-1/2 within the KKR DFT. We find that both the lattice parameter and the indirect band gap satisfy Vegard's law including a bowing parameter.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). <https://doi.org/10.1103/PhysRevB.88.094421>

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. 65, 353 (1990). <https://doi.org/10.1103/PhysRevLett.65.353>

[3] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). <https://doi.org/10.1103/PhysRevB.78.125116>

MM 6.7 Mon 17:30 H44

**Using MD simulations to better understand and control self-propagating reactions in Al-Ni multilayers** — ●FABIAN SCHWARZ and RALPH SPOLENAK — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Reactive multilayers are capable of releasing large amounts of heat in a short time, making them a possible tool for energy storage or joining applications. Molecular Dynamics (MD) simulations can be used as a tool to study the front propagation, while varying certain system parameters. We study the influence of the crystal structure on the reaction front propagation in Al-Ni multilayers by looking at various microstructures, such as amorphous, single crystal or different grain structures. We found that crystallinity has a significant impact on the front propagation speed, which is likely related to different diffusion mechanisms. The more disordered the individual layers become, e.g., by increasing the grain boundary density, the higher is the resulting propagation speed. Furthermore, we study the influence of a premixed interlayer at the interface on the reaction propagation. For this, premixed interlayers with different, namely homogeneous, gradient and s-shaped profiles are studied and compared to existing experimental results. Beyond better understanding of the premixed interlayer, we show that it can be used to control the front propagation speed in reactive multilayers. Furthermore, we show that the heat of crystallization of amorphous AlNi to B2-AlNi alone is high enough for a self-propagating reaction to occur.

MM 6.8 Mon 17:45 H44

**strong impact of spin fluctuations on the antiphase boundary energies of weak ferromagnetic Ni<sub>3</sub>Al** — ●XIANG XU<sup>1,2</sup>, XI ZHANG<sup>2</sup>, ANDREI RUBAN<sup>3,4</sup>, SIEGFRIED SCHMAUDER<sup>1</sup>, and BLAZEJ GRABOWSKI<sup>2</sup> — <sup>1</sup>Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Germany — <sup>2</sup>Institute for Materials Science, University of Stuttgart, Germany — <sup>3</sup>KTH Royal Institute of Technology, Stockholm, Sweden — <sup>4</sup>Materials Center Leoben Forschung GmbH, Leoben, Austria

The antiphase boundary (APB) was believed to be crucial for explaining the anomalously increased yield stresses of  $\text{L1}_2$   $\text{Ni}_3\text{Al}$ . However, an accurate temperature-dependent APB energy is still missing and the magnetic effect was often underestimated or even neglected. In this work, the influence of longitudinal spin fluctuations (LSF) as well as other thermal mechanisms were considered within the ab-initio framework up till the melting point. We found that the calculated  $T$ -dependent APB energies show a remarkable agreement with the experimental data despite the large discrepancy between different works. The LSF effect was determined to crucially increase APB energies, especially for (100)APB with a maximum of 50% over the nonmag-

netic data. This significant contribution prompts to take serious consideration of LSFs when studying the paramagnetism, even for weak itinerant ferromagnetic materials. The accurate APB energy acquired in this work can be used to set up quantitative models for simulating dislocation motions and the elastic-plastic behavior for Ni-based superalloys on the macro scale.

MM 6.9 Mon 18:00 H44

**Ab initio study on the phase stabilities of multi-component carbides in high-Mn steels** — LEKSHMI SREEKALA<sup>1</sup>, JÖRG NEUGEBAUER<sup>1</sup>, and ●TILMANN HICKEL<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — <sup>2</sup>BAM Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

The high strength and ductility of advanced high Mn steels makes them suitable for lightweight applications in the transportation sector. A modification of their properties can be achieved by intentional or unintentional addition of further alloying elements, which is often connected with the formation of secondary phases. In particular, Cr addition improves corrosion resistance and, at the same time, inadvertently yields a substantial increase in the number of carbides precipitated, such as  $\text{Fe}_3\text{C}$  and  $\text{Fe}_{23}\text{C}_6$ . Therefore, in the present work, we use density functional theory to determine the thermodynamic driving force for the formation of these multicomponent carbides by evaluating their phase stabilities. We study the free energy of formation at finite temperatures by considering the vibrational, electronic and magnetic contributions. While both Cr and Mn stabilize Fe-carbides, we found that the impact of Cr is higher than that of Mn for a typical host matrix composition of Fe, Cr and Mn. Further, we analyze the critical role of magneto-structural coupling for the phase stability of these compositionally complex carbides. Through this study, we demonstrate the predictive capability of ab initio thermodynamics to accurately describe the phase stabilities of chemically complex secondary phases in metallic alloys.

MM 6.10 Mon 18:15 H44

**Atomistic simulation of diffusion in  $\gamma'$ -strengthened Co-based superalloys** — ●LIN QIN<sup>1</sup>, JUTTA LOGAL<sup>2,3</sup>, DOROTA KUBACKA<sup>4</sup>, and RALF DRATZ<sup>1</sup> — <sup>1</sup>ICAMS, Ruhr University Bochum, Bochum, Germany — <sup>2</sup>Department of Chemistry, New York University, New York, United States — <sup>3</sup>Department of Physics, Free University of Berlin, Berlin, Germany — <sup>4</sup>Institute of Micro- and Nanostructure Research, FAU, Erlangen, Germany

The suppressed diffusion of Al in the strengthening  $\gamma'$  precipitates in Co-based superalloys is suspected to be one plausible reason to cause the selective formation of alumina in the early stage of oxidation above 900°C. In order to validate this assumption, the diffusion properties of Al, Co and W in a prototype structure of  $\gamma'$  phase, i.e.  $\text{L1}_2\text{-Co}_3(\text{Al}, \text{W})$ , are investigated with Density Functional Theory (DFT) and Kinetic Monte Carlo (KMC) simulations. DFT calculations reveal that the migration barrier of each element in Co sublattice is comparable with its respective barrier in pure Co. However, the crossover barriers of Al and W from their original positions to Co sublattice are much higher than the barriers for the reverse process. This large discrepancy in barriers constrains the site fraction of Al and W in Co sublattice, and therefore significantly suppresses the long-distance diffusion of Al and W in  $\gamma'$  phase. KMC results show that Al diffusivity in  $\gamma'$  phase is over two orders of magnitude lower than that in a solute  $\gamma$  phase ( $\text{Co}_{75}\text{Al}_{12.5}\text{W}_{12.5}$ ) at 900°C, suggesting that the sluggish diffusion of Al in  $\gamma'$  can be a possible reason to cause the selective formation of alumina in Co-based superalloys.