MM 41: Topical Session: Defect Phases III

Time: Thursday 15:45–18:00 Location: SCH A 216

Topical Talk MM 41.1 Thu 15:45 SCH A 216

Entropy in grain boundary segregation — •Pavel Lejcek — CEITEC, BUT, Brno, Czechia — Institute of Physics, AS CR, Prague Czechia

Experimentally, a linear dependence between the standard entropy and the standard enthalpy of solute segregation at grain boundaries was established which is called *enthalpy-entropy compensation effect*. In this dependence, there exists a region in which the product of temperature and segregation entropy ('entropy term') is larger than the absolute value of the segregation enthalpy, so that the controlling parameter, the Gibbs energy of segregation, is negative. Under this condition the grain boundary segregation is dominated by the entropy, i.e., the phenomenon of the entropy-dominated grain boundary segregation occurs. We show numerous examples of the grain boundaries and solutes in bcc-iron-based alloys exhibiting this phenomenon. In addition, we formulate the idea that a solute can also segregate at the grain boundary (site) that exhibits positive segregation energy/enthalpy (so called *anti-segregation site*) if the entropy term is larger than the segregation enthalpy, so that the Gibbs energy o segregation is negative. In this way, the solute segregation is completely controlled by the entropy term and an entropy-driven grain boundary segregation will exist. We suggest the entropy-driven grain boundary segregation for several model examples in iron-based systems thus serving as indirect evidence of the phenomenon. Finally, the grain boundary configurational entropy is discussed in relation to its volume counterpart and to the segregation variables.

MM 41.2 Thu 16:15 SCH A 216

Impact of precipitation on grain boundary diffusion in microstructure-engineered Ni-Cr-Fe alloy — •Baixue Bian, Mohan Muralikrishna Garlapati, Shabnam Taheriniya, Sandipan Sen, Gerhard Wilde, and Sergiy V. Divinski — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Gemany

Grain boundary structure-property relationship is studied in a Ni-based Inconel 602CA coarse-grained alloy using a novel correlative tracer diffusion-analytical microscopy approach. Homogenized and intermediate-annealed states are used to engineer the alloy microstructure. Grain boundary diffusion of Ni and Cr is measured in both C- and B-type kinetic regimes. A co-existence of several short-circuit contributions to tracer diffusion is distinguished and correlated to distinct grain boundary precipitation and segregation as revealed by HAADF-STEM combined with EDX measurements. The homogenized state reveals precipitation of Ni-based L12 and Cr23C6 phases which influence significantly diffusion properties. The intermediate annealing promotes a uniform formation of Cr carbides with a minimal/negligible fraction of the L12 phase. The present study demonstrates the correlated structure-kinetic property measurements provide a unique tool to probe the grain boundary precipitation in these industrially used Inconel alloys.

MM 41.3 Thu 16:30 SCH A 216

Orientation relationship and interface inclination in dependence of heat treatment time between Al2Ca and Mg Matrix — •Lukas Berners[1], Zhuocheng Xie[1], Mattis Seehaus[1], Siyuan Zhang[2], and Korte-Kerzel Sandra[1] — [1]IMM, RWTH Aachen — [2]MPIE, Düsseldorf

Mechanical properties of two phase-alloys are highly dependent on the morphology of the second phase as well as the interface character. Analysis of the orientation-relationship between the magnesium matrix and C15 (Al2Ca) Laves phase precipitate is up to now mainly conducted via TEM analysis. However, where defect phases as thermodynamically stable interface configurations are to be identified, a more statistically significant approach is needed. To this end, we use large scale EBSD to reveal prevalent orientation relationships as well as interface character during the transition from hexagonal C36 phase to cubic C15 phase during heat treatment at 500 °C and thus unravelling a pathway to the thermodynamically stable interface configuration.

MM 41.4 Thu 16:45 SCH A 216

Non-Arrhenius temperature dependence of grain boundary diffusion in additively manufactured high-entropy CoCrFeMnNi alloy — •Nuri Choi[1], Manoel W. da Siva Pinto[1], Saba Khademorezaian[1], Sangsun Yang[2], Ji Hun Yu[2], Jai Sung Lee[3], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Material Physics, University of Münster, Münster, Germany — [2]Center for 3D Printing Materials Research, Korea Institute of Materials Science, Changwon, South Korea — [3]Dep. of Mat. Sci. & Chem. Eng., Hanyang University, Ansan, South Korea

Additive manufacturing process induces numerous crystalline defects such as vacancies, dislocations and dislocation networks, non-equilibrium segregation which affect mechanical, kinetic and structural properties of the fabricated materials. Moreover, a non-equilibrium state of grain boundaries has been discovered, too, which is characterized by enhanced rates of grain boundary diffusion at relatively low temperatures [1]. In the present study, grain boundary diffusion of Ni in additively manufactured CoCrFeMnNi high-entropy alloys is measured in an extended temperature interval. A non-monotonous temperature dependence is observed and interpreted in terms of a thermally-activated relaxation of the non-equilibrium state. The grain boundary energy is evaluated from the grain boundary diffusivity data for various heat-treatment conditions and compared to the total energy released during annealing by differential scanning calorimetry. The evolution of microstructure and mechanical properties is discussed, too.

15 min. break

MM 41.5 Thu 17:15 SCH A 216

Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases — •Zhuocheng Xie[1], Dimitri Chauraud[2], Achraf Atila[2,3], Erik Bitzek[2,3], Sandra Korte-Kerzel[1], and Julien Guénolé[4,5] — [1]Institute of Physical Metallurgy and Materials Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [3]Department of Materials Science and Engineering, Institute I: General Materials Properties, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, 57070 Metz, France — [5]Labex Damas, Université de Lorraine, 57070 Metz, France

Synchroshear as the dominant basal slip mechanism in Laves phases is accomplished by the glide of synchro-Shockley dislocations. However, the mechanism of synchro-Shockley dislocation motion is still not well understood. In this work, we demonstrate kink propagation as the energetically favorable mechanism for the motion of synchro-Shockley dislocation using atomistic simulations. Vacancy hopping and interstitial shuffling are identified as two key mechanisms of kink propagation. The assistance of vacancy and antisite defects on kink nucleation and propagation are investigated and shown crucial for kink mobility. These findings provide insights into the dependency on temperature and chemical composition of plastic deformation of topologically close-packed phases.

MM 41.6 Thu 17:30 SCH A 216

Defect bulk-boundary correspondence of topological skyrmion phases of matter — •Shuwei Liu[1,2], Likun Shi[1], and Ashley M. Cook[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, — [2]Max Planck Institute for Chemical Physics of Solids

Unpaired Majorana zero-modes are central to topological quantum computation schemes as building blocks of topological qubits, and are therefore under intense experimental and theoretical investigation. Their generalizations to parafermions and Fibonacci anyons are also of great interest, in particular for universal quantum computation schemes. In this work, we find a different generalization of Majorana zero-modes in effectively non-interacting systems, which are zero-energy bound states that exhibit a cross structure, two straight and perpendicular lines in the complex plane, composed of the complex number entries of the zero-mode wavefunction on a lattice, rather than a single straight line formed by complex number entries of the wavefunction on a lattice as in the case of an unpaired Majorana zero-mode. These *cross* zero-modes are realized for topological skyrmion phases under certain open boundary conditions when their characteristic momentum-space spin textures trap topological defects. In the

process of characterizing this defect bulk-boundary correspondence, we develop recipes for constructing physically-relevant model Hamiltonians for topological skyrmion phases, efficient methods for computing the skyrmion number, and introduce three-dimensional topological skyrmion phases into the literature.

MM 41.7 Thu 17:45 SCH A 216

Ga Induced Defect Phase Transformations in the Σ7 Mg Grain Boundary — •Prince Mathews[1], Siyuan Zhang[1], Christina Scheu[1], Tilmann Hickel[1,2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf — [2]Federal Institute for Materials Research and Testing (BAM), D-12489 Berlin, Germany

The design of tailored materials requires to understand not only bulk phases but also the stability of various defect phases. Grain boundaries (GBs) form one class of defects that directly influence the properties of the material. Therefore, GB phase transformations introduced by alloying can alter mechanical performance. In this work, the Σ7 [0001] | 21.78° (sym. plane 12-30) GB in hcp Mg is investigated, for which an A- and a T-type is known. Ab-initio simulations as a function of stress and temperature (using quasi-harmonic approximation) are performed, and show the presence of a phase transformation. Based on the computed Gibbs energies, the defect phase diagram as a function of the Ga chemical potential is determined. To this end, a complete set of Ga configurations at the GB is first screened with an empirical potential, before accurate ab initio calculations are performed for the low-energy configurations. Ga is not only found to trigger a transformation between T and A type, but a systematic transition of the preferred segregation sites is also seen with an increasing number of Ga atoms at the GB. The results qualitatively agree well with experimental results from high-resolution transition electron microscopy (HR-TEM). Physical mechanisms are provided to explain remaining discrepancies.