MM 13: Topical Session: Defects of Defects

Time: Tuesday 14:00–15:30 Location: H10

Topical Talk MM 13.1 Tue 14:00 H10

Dynamics of dislocations and grain boundaries during recrystallization of metal nanoparticles — •Eugen Rabkin and Jonathan Zimmerman — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa, Israel

Recrystallization of bulk metals plays a central role in materials processing, yet it has not been utilized so far for the synthesis of metal nanoparticles. In this work we describe the kinetics of recrystallization and related annealing phenomena in Pt nanoparticles. We uniaxially deformed the particles, annealed them both in-situ and ex-situ, and characterized their morphology and microstructure. Our findings reveal that new grains often nucleate within the parent particle, only to be rapidly reabsorbed back into it, with a strong correlation between this phenomenon and particle size. We propose a model that combines recrystallization and recovery through dislocation annihilation at the particle surface, predicting a critical size for recrystallization in nanoparticles. Finally, we propose a set of rules for nanoparticle recrystallization, mirroring the rules of recrystallization in bulk materials.

MM 13.2 Tue 14:30 H10

Hierarchy of defects in near-Σ5 tilt grain boundaries in copper studied by length-scale bridging electron microscopy — •Hui Ding[1], Anoosheh Akbari[2], Enze Chen[3], Harald Rösner[2], Timofey Frolov[4], Sergiy Divinski[2], Gerhard Wilde[2], and Christian H. Liebscher[5] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]University of M\"unster, Institute of Materials Physics, Münster, Germany — [3]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA — [4]{Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — [5]Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

Grain boundaries (GBs) are material imperfections that significantly impact material properties. In this study, we utilized aberration-corrected scanning transmission electron microscopy to examine the structure of a series of near- Σ5(310)[001] tilt grain boundaries in copper. Globally, the GB appears flat with no noticeable defects. On the atomic-scale, however, various types of GB defects are observed. When a slight deviation in the misorientation is introduced, a patterning emerges featuring characteristic structural units from the Σ5 (310) [001] and Σ5 (210) [001] tilt boundaries. The structural landscape of the GB becomes more complex when GB plane inclination is also present, such as a wavy morphology or staircase-like architecture. Our investigation into GB structure, particularly its inherent defects, is a prerequisite towards gaining atomic-scale insights into their potential impact on material properties.

MM 13.3 Tue 14:45 H10

Data-driven modelling of vacancy segregation to grain-boundaries — •Christoph Dösinger, Oliver Renk, and Lorenz Romaner — Montanuniversität Leoben, Department of Materials Science, Roseggerstraße 12, A-8700 Leoben, Austria

Both vacancies and grain-boundaries (GB) are important defects in materials. The vacancies can interact with the GBs which might lead to a formation of voids, as a result this might start the formation of pores or cracks. From atomistic simulations it is known that vacancies can be attracted to GBs, which indeed may act as sinks for the vacancies. However, such simulations, especially if performed using ab-initio, methods can be tedious and costly. In this work we apply machine learning (ML) methods to predict the segregation energies of vacancies to GBs, which give a measure how strongly a vacancy is attracted to specific sites at different GBs. For this ML approach each segregation site is described by its local environment which can be encoded by using for example Steinhardt or SOAP parameters. Together with the site-specific segregation energies a regression model, in our case a Gaussian Process, is trained. Previously we have shown that this approach can be used to predict the segregation of solutes to grain-boundaries. This method for prediction the segregation of vacancies is tested and applied to GBs in tungsten, for which a complete data-set is available for 15 different GBs ($\Sigma3 - \Sigma43$). By using this diverse set of GBs, it will be possible to predict the GB segregation of vacancies for general GBs or polycrystalline materials.

MM 13.4 Tue 15:00 H10

A high-throughput ab initio segregation study of light elements at Ni grain boundaries and their effects on cohesion — •Han Lin Mai[1], Jörg Neugebauer[1], and Tilmann Hickel[2] — [1]Max-Planck-Institut for Nachhaltige Materialien GmbH, Dusseldorf, Germany — [2]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany

Segregation of alloying/tramp elements to grain boundaries (GBs) can drastically affect the properties of metallic alloys. We present a high-throughput density-functional theory-based study on the segregation of smaller elements, H, B, C, N, O, P, S, in a variety of FCC Ni GBs and their effects on cohesion. To support GB engineering efforts, we investigate the thermodynamics of segregation and calculate its effects on interface cohesion. These elements often play a significant role in engineering alloys, but their positioning at GBs is ambiguous and challenging to study. The study utilizes efficient and highly automated workflows using the integrated development environment pyiron. We discuss chemical and structural trends for segregation and cohesion at GBs for these elements. In order of segregation binding strength at GBs, the trend is approximately $O > B, S > P > N = C = H$. Elemental trends for maximum segregation binding strength across various GB models are largely consistent, enabling qualitative cross-element comparisons through small GB sets. However, conventional metrics, such as GB energy, are insufficient for predicting segregation strength or quantity for these elements.

MM 13.5 Tue 15:15 H10

Mechanistic Influence of Interstitial Solutes on Hydrogen Trapping at Σ5 GB in γ-Fe — •Poulami Chakraborty, Mauricio Rincon Bonilla, and Elena Akhmatskaya — Basque Centre for Applied Mathematics, Bilbao, Spain

The local variation of grain boundary atomic structures and chemistry caused by segregation of impurities influences the macroscopic properties of polycrystalline materials. Here, the effect of co-segregation of carbon and boron on hydrogen segregation at a Σ5 (210) [001] tilt grain boundary in γ-Fe phase is studied by density functional theory. The grain boundary structure predominantly features kite-like motifs, which are disrupted by atomic-scale defects. First-principles calculations indicate that carbon and boron exhibit the strongest segregation tendency. Their interaction with aluminum is notably repulsive, leading to aluminum depletion at the grain boundary. Subsequently, the effect of boron and carbon co-segregation is studied with the introduction of H at the GB. Our comprehensive investigation provides valuable insight in the interaction of interstitial impurities with substitutional solutes, which, strongly influences grain boundary composition and the properties of the interface.