MM 54: Topical Session: Interface-dominated phenomena - Crystallization and Microstructure Evolution

Time: Thursday 11:45–12:45 Location: IFW A

MM 54.1 Thu 11:45 IFW A

Atomistic investigation of phase boundary migration during solid-solid phase transformations in tungsten — •Yanyan Liang, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The phase transformation between the topological close packed A15 and cubic BCC in the transition metal tungsten has recently incited attention, given the applications in microelectronics and spintronic devices where either BCC or A15 is favourable. The underlying atomistic processes greatly influence the kinetics of phase transformations, specifically the mobility and corresponding growth velocity of interfaces. At high temperatures, phase boundary migration can be captured by conventional molecular dynamics (MD) simulations. At moderate temperatures, however, enhanced sampling techniques are required due to the slow movement of the interface and corresponding extended timescales that need to be covered. We combine both, high-temperature MD and low-temperature enhanced sampling, to investigate phase boundary migration between A15 and BCC in W. From these simulations, we extract information concerning the growth mode, such as step nucleation and growth along the step edges or island formations. Furthermore, we investigate the influence of driving forces on interface migration at different mismatches between A15 and BCC. Together with the evaluation of energy barriers connected to the migration of the phase boundary, we provide novel insight into the atomistic mechanism and kinetics during the solid-solid phase transformation.

MM 54.2 Thu 12:00 IFW A

A study of texture controlled grain growth in thin films by 3D simulations — •Dana Zöllner and Igor Zlotnikov — B CUBE - Center for Molecular Bioengineering, TU Dresden, Tatzberg 41, 01307 Dresden

Historically, metallography used to be the purely two-dimensional characterization of the microstructure of materials by optical microscopy. The main problem: A 2D section through a complex three-dimensional entity gives us only a poor description of the true size and shape. Therefore, numerous attempts have been made to obtain full three-dimensional structural information experimentally. Nevertheless, in computer simulations as well as analytical theories coarsening in thin films is frequently treated as a two-dimensional process still today. In the present investigation, grain growth in thin films is modeled by three-dimensional Potts model simulations focusing on the influence of initial texture associated with the grain microstructure. Different initial crystallographic textures yield different spatial distributions of boundary mobilities in the grain boundary network leading to a diversity of coarsening kinetics.

MM 54.3 Thu 12:15 IFW A

Shedding light on polymorph selection and seeding mechanisms during crystal nucleation in metals — •Grisell Díaz Leines and Jutta Rogal — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum, Germany

Fundamental knowledge of the mechanism and the principles of polymorph selection during crystal nucleation is essential for the synthesis and control of materials with targeted properties. However, understanding the atomistic mechanism of crystallization poses a major challenge as many materials exhibit complex transitions with multiple steps, forming polymorphic structures. Here, we employ an advanced atomistic simulation method, transition path sampling, to investigate the formation mechanism of crystal clusters during homogenous and heterogeneous nucleation in metals. The analysis of the nucleation pathways in Ni shows that the formation of pre-ordered liquid regions with increased bond-orientational order facilitates the emergence of crystallites by decreasing the interfacial free energy. The pre-structured cloud acts as a precursor of crystallization and predetermines the polymorph selected. Furthermore, we explore how selected crystal seeds influence the polymorphic outcome and efficiency of the nucleation process in Ni. Our investigation reveals a novel mechanism of heterogeneous nucleation, demonstrating that the ability of small seeds to promote bond-orientational order fluctuations and template the formation of effective precursors in the liquid, is central to understand the enhancement of the nucleation probability and the selection of polymorphs during crystallization.

MM 54.4 Thu 12:30 IFW A

Impurity effect on microstructure homogeneity, recrystallization kinetics and mechanical properties in severe plastically deformed coppers — •Yao Jiang[1,2], Martin Peterlechner[2], Ruicong Gu[1], Jingtao Wang[1,3], and Gerhard Wilde[2,3] — [1]School of Materials Science and Engineering, Nanjing University of Science and Technology, 210094 Nanjing, P.R. China — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany — [3]Herbert Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, 210094 Nanjing, P.R. China

Recrystallization and mechanical behavior of ultra-fine grained (UFG) copper prepared by equal channel angular pressing and nano-lamellar (NL) copper by ECAP with additional cryogenic rolling were investigated by comparing coppers with two different purity of 4N and 3N. Discontinuous nucleation and grain growth were observed to be uncorrelated to shear bands. The discontinuous recrystallization was considered to modify JMAK model and to quantify the microstructure inhomogeneity. Moreover, the thermal stability of the NL structure was comparable to the UFG structure, due to their similar activation energy for recrystallization. Superior strength and ductility was achieved in the partially recrystallized NL structural 3N copper. The present work proposed an effective strategy to tailor the nuclei sites and grain growth of the partial recrystallization by using localized shear bands and composition.