

MM 1: Invited talk Liebscher

Time: Monday 9:30–10:00

Location: BAR 205

Invited Talk

MM 1.1 Mon 9:30 BAR 205

Atomic resolution observations of grain boundary phase transformations — •CHRISTIAN LIEBSCHER¹, THORSTEN MEINERS¹, NICOLAS PETER¹, TIMOFEY FROLOV², ROBERT RUDD², and GERHARD DEHM¹ — ¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — ²Lawrence Livermore National Laboratory, Livermore, USA

The theory that grain boundaries (GBs) can undergo phase transformations has a long history. More than 50 years ago, thermodynamic concepts have been established that GBs can exist in multiple phase states. It was assumed that stable and metastable states exist for different GB orientations. Only indirect measurements have indicated the existence of interfacial transitions and the search for these GB phases

has been in vain.

Here, we present atomic resolution insights into grain boundary phase transformations and how they influence the interfacial properties. We combine advanced scanning transmission electron microscopy with atomistic simulations to resolve the atomic structure of GB phases and explore their atomistic and thermodynamic properties. We will show examples how nanoscale faceting transitions can either lead to anomalous segregation behavior or are triggered by solute segregation in both semiconductors and alloys. Even in elemental copper, we observe grain boundary phase coexistence at symmetric and asymmetric GBs. Evolutionary GB search finds the same structures as in experiment and finite temperature molecular dynamics simulations explore their transformation behavior.