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ABSTRACT:

Grain Boundary Phase Transformations and Segregation Transitions in Metallic Alloys

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Grain boundaries (GBs) are one of the most ubiquitous defects in metallic materials and largely impact materials properties and functionality. More than 60 years ago following thermodynamic concepts, it was proposed that GBs themselves can transform from one state into another by changing temperature or pressure [1]. With the advent of new computational tools and approaches it was shown that GBs in different material systems, such as copper (Cu) and tungsten, can exist in multiple stable and metastable states [2,3]. However, direct experimental observations remained challenging, because of the confined nanoscale nature of GBs and their complex atomic arrangements.

I will show by a combination of atomic resolution scanning transmission electron microscopy (STEM) and atomistic modelling that two GB phases can undergo phase transformation in elemental Cu in a S19b [111] [4]. Finite temperature molecular dynamics simulations indicate that a new line defect, the grain boundary phase junction, separating the pearl and domino GB phases is kinetically limiting the phase transformation making room temperature observations possible.

In a related S37c [111] tilt GB, I will show observations of GB phases arranging themselves in a periodic manner with nanometer sized segments of the pearl and domino phases [5]. An exploration of the nucleation and growth conditions indicates that also here the grain boundary phase junction plays a decisive role in the GB phase arrangement. I will further show direct observations of GB phase transformation on the atomic scale by *in situ* heating experiments in the STEM.

In the last part of the talk, I will give an example of a segregation induced GB transition in [0001] tilt GBs in titanium induced by iron (Fe). Here, solute segregation of Fe leads to the formation of cage-like icosahedral structures that represent a new structural state of the GB, which is indicative of a segregation induced GB transition.

[1] E.W. Hart *et al.*, Scr. Metall. 2, 179–182 (1968)
[2] Q. Zhu *et al.*, Nat. Commun. 9, 1–9 (2018)
[3] T. Frolov *et al.*, Nanoscale 10, 8253–8268 (2018)
[4] T. Meiners *et al.*, Nature 579, 375–378 (2020)

[5] L. Langenohl *et al.*, Nat. Commun. 13, 3331 (2022)