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ABSTRACT:

Atomistic Modeling of the Thermodynamics of Grain Boundaries in fcc Metals

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Grain boundaries (GBs) influence many macroscopic material properties—such as strength, toughness, or grain growth—and can act as fast pathways for diffusion, often leading to segregation. In recent years, interest in the atomic structure of GBs has grown and transmission electron microscopy (TEM) imaging has helped to prove the (co-)existence of so-called “complexions” or “GB phases”, which have long been predicted by theory and simulation: Different atomic structures at the same GB can be treated as the 2D analogue of bulk phases, GB phase diagrams can be constructed, and GB phase transitions can be observed. These seemingly minute details have already been shown to influence, e.g., the diffusion coefficient in copper [1,2]. Here [3], we focus on atomistic simulations using EAM potentials on ⟨111⟩ tilt GBs in fcc metals, where we could—together with TEM experiments—identify three families of GB phases, dubbed “domino”, “pearl”, and “zipper”, e.g., at Σ37c GBs in Cu [4] and Al. Interestingly, GB phase transitions between pearl and domino can already be observed as a function of temperature or stress in pure materials [4]. Using simulations, we could show for a range of fcc metals that domino and pearl are universal to this material class [5]. The GB structures are related to the crystal structure, but the energetics and thermodynamics are material dependent [5]. Real world materials, however, are never pure and segregation can influence the properties of the GB and can even trigger GB phase transitions. We show how segregation of Ag to Cu GBs proceeds at an atomic level for the zipper [6] and domino/pearl phases. We highlight that the segregation process is strongly influenced by the structure on the atomistic level and therefore sensitive to GB phase transitions.

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