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ABSTRACT:

Transitions in Grain Boundary Migration and the Effect of Grain-Scale Elastic Constraints

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Grain boundary (GB) migration in polycrystals is influenced by various factors, including temperature, driving force, boundary character, defects, and constraints imposed by polycrystalline systems. Molecular dynamics studies in bicrystals routinely investigate the role of temperature, driving force, boundary character. This study examines these behaviors in the context of the recently hypothesized Kosterlitz-Thouless (KT) topological transition [1]. This KT transition emerges at elevated temperature when disconnection pairs become unbound, leading to changes in migration behaviors. Specifically, we examine changes in mobility, shear coupling, and boundary roughness and compare these across six special and general GBs.

This study also includes efforts to investigate grain-scale elastic constraints present in polycrystalline systems. The method introduces an elastic restoring force (related to grain size) in response to lateral motion induced by shear coupling. In a sampling of 20 special and general GBs, the constraints lead to a variety of responses, including shear coupled mode switching or a complete cessation of migration. The constraints leave mobility largely unaffected in some GBs, but in others, mobility is significantly reduced, particularly at low temperatures and driving forces.

[1] K. Chen, D.J. Srolovitz, and J. Han, Proc. Natl. Acad. Sci. 117, 33077 (2020).