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Stiffness Matters: The Role of the Interface Stiffness Tensor on Grain Boundary Dynamical Processes

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Many problems in materials science involve free and/or moving boundaries. When solving these at the mesoscopic scale, sharp interface equations are typically derived to describe interfacial dynamics, where the interface properties are key input parameters. Herein and based on theoretical analysis, and mesoscale and atomistic simulations, we show that when considering the grain boundary (GB) inclination degrees of freedom the GB interface stiffness tensor plays a paramount role in a wide range of GB dynamical processes. Eigenvalue analysis of the stiffness tensor of several GBs reveals that the stiffness is much larger in magnitude and more anisotropic than the energy itself, and for some inclinations is negative indicating a propensity to break up into facets. In broad terms, our analysis and simulation results provide future avenues to explore the role of GB stiffness on microstructural evolution problems.

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