

Continuum modeling of disconnection-mediated interface migration in crystals

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The migration of interfaces in crystalline materials, such as grain boundaries, is governed by mechanisms that reflect the underlying lattice structure. While the reduction of interface energy provides a fundamental thermodynamic driving force, it alone cannot account for several essential physical effects. A key phenomenon in this context is the coupling between interface migration and shear deformation (shear coupling), which leads to the buildup of internal stresses and mediates the response of crystalline systems to applied stress. At the microscopic level, this behavior can be ascribed to the motion of disconnections, i.e., line defects confined to interfaces possessing both step and dislocation character. Connecting such a microscopic mechanism to macroscopic evolution requires appropriate coarse-graining and mesoscale modeling.

In this seminar, a continuum formulation capturing disconnection-mediated interface migration within a self-consistent, crystallography-respecting framework will be presented. The basic model, which links interface geometry to disconnection density and describes disconnection flow as driven by both interface-energy reduction and applied or internal stresses, will be outlined. Extensions of the model will then be illustrated alongside applications, including the role of internal stresses in interface faceting and the link between multimode disconnection flow (disconnections with multiple step heights) and grain rotation. The modeling challenges and the resulting mathematical formulations will be discussed, along with a diffuse-interface (phase-field) formulation of the continuum model enabling advanced simulations. Finally, combining the proposed continuum formulation with multiphase-field modeling will show that disconnection-mediated shear coupling drives grain growth in crystalline systems beyond the classical curvature-driven paradigm.