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Continuum Models for Structures and Dynamics of Interfaces in Crystalline Materials

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Interfaces in crystalline materials are planar defects across which grains have different orientations (grain boundaries), or the material composition and/or crystal lattice structure changes (hetero-interfaces). Structural and dynamic properties of interfaces play essential roles in the mechanical and plastic behaviors of the materials. These properties of interfaces strongly depend on their microscopic structures. We present continuum models for the structures and dynamics of interfaces in crystalline materials based on the continuum distribution of the line defects (dislocations or disconnections) on them. Numerical simulations based on our models are performed and compared with experiments and atomistic simulations, which shows the excellent predictions.