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Resolving Self-Stress Artifacts in Twin Boundary Migration: A Stress Correction Scheme for the CPFE-PF Model of HCP Alloys

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ABSTRACT

The plastic deformation of Mg/Ti alloys arises from the synergistic interplay of dislocation slip and deformation twinning. To model these mechanisms, we previously developed a mesoscale CPFE-PF framework that couples crystal plasticity finite element (CPFE) and phase field (PF) methods, enabling predictions of microstructure evolution and mechanical behavior under complex loading. A central challenge, however, lies in accurately capturing deformation twinning—a process critical for accommodating shear and reorienting crystal domains in low-symmetry metals. Twin propagation and thickening occur via twinning dislocations/disconnections at the atomic scale, while at larger scales they are governed by the migration of twin boundaries. Mesoscale twin boundary migration in conventional PF models is distorted by artificial self-stress effects. These spurious stresses, inherent to continuum approaches, stem from singular or discontinuous stress fields at interfaces, leading to unphysical driving forces and erroneous predictions of twin growth. To address this limitation, we introduce a stress correction scheme that isolates and suppresses self-stress artifacts at twin boundaries. By analyzing 3D twin stress fields (sharp and diffuse interface) through dislocation theory and CPFE simulations, we define a "correction zone" to recalibrate the interface driving force. The method interpolates bulk stress values outside this zone, effectively approximating the true mechanical driving force while filtering out self-stress contributions. Validation within the CPFE framework confirms a significant reduction in spurious forces. We then integrate this scheme into the CPFE-PF model to simulate dynamic 3D twin evolution in Mg alloys. Results demonstrate that the corrected model eliminates unrealistic interface migration behavior observed in self-stress-driven scenarios, achieving closer alignment with physical twin evolution mechanisms.

KEYWORDS

Deformation twin; self-stress; phase field; crystal plasticity finite element

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