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Phase Field Crystal Simulation of Mechanical Properties and Grain Boundary Evolution of Complex Concentration Alloys

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ABSTRACT

The complex concentration alloys are considered to have excellent mechanical properties due to the combined effects of heterogeneous composition and microstructure. However, it is difficult for existing simulation methods to capture the significant modulation of mechanical properties by the formation and motion of grain boundaries of complex concentration alloys at the microsecond and nanometer scales. To address this, we utilize the phase field crystal model that combines molecular dynamics and traditional phase field advantages to systematically study real-time grain boundary formation and motion in complex concentration alloys [1]. Meanwhile, we investigated the compositional fluctuations of low concentration alloys at grain boundaries and during long-term grain growth processes. In addition, we investigated the effects of concentration gradients in complex concentration alloys on grain rotation and coalescence, as well as the effects of compositional fluctuations on lattice distortion and dislocation motion during deformation. This study can provide a deeper understanding of the real-time atomic scale complex concentration alloy grain boundary evolution mechanism.

KEYWORDS

Complex concentration alloy; grain boundary; phase field crystal; composition undulation

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