Structural Disjoining Potential for Grain Boundary Premelting and Grain Coalescence from Molecular-Dynamics Simulations

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Abstract

We describe a molecular dynamics framework for the direct calculation of the short-ranged structural forces underlying grain-boundary premelting and grain-coalescence in solidification. The method is applied in a comparative study of (i) a $\Sigma 9$ $\langle 115 \rangle$ 120^o twist and (ii) a $\Sigma 9$ $\langle 110 \rangle$ $\{411\}$ symmetric tilt boundary in a classical embedded-atom model of elemental Ni. Although both boundaries feature highly disordered structures near the melting point, the nature of the temperature dependence of the width of the disordered regions in these boundaries is qualitatively different. The former boundary displays behavior consistent with a logarithmically diverging premelted layer thickness as the melting temperature is approached from below, while the latter displays behavior featuring a finite grain-boundary width at the melting point. It is demonstrated that both types of behavior can be quantitatively described within a sharp-interface thermodynamic formalism involving a width-dependent interfacial free energy, referred to as the disjoining potential. The disjoining potential for boundary (i) is calculated to display a monotonic exponential dependence on width, while that of boundary (ii) features a weak attractive minimum. The results of this work are discussed in relation to recent simulation and theoretical studies of the thermodynamic forces underlying grain-boundary premelting.