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Atomistic characterization of solid–liquid interfaces in Cu–Ni binary system

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ABSTRACT

The study of microscopic structure, dynamics, and thermodynamics of solid–liquid interfaces is of vital importance to the understanding of a series of phenomena, e.g., the dendrite growth in pure metals or alloys. However, direct experimental observations of the solid–liquid interfaces are still difficult and rare. As a result, most of the information on the microscopic structure and thermodynamics of solid–liquid interfaces was obtained from atomistic simulations. In the present work, the structural and dynamical properties of the solid–liquid interfaces in a Cu–Ni alloy with different orientations of the solid, i.e., (100), (110), and (111) were examined by molecular dynamics simulations based on an embedded-atom-method potential. The profiles of local order parameter, atomic number density, and diffusion coefficients were evaluated to determine the interfacial width. It is found that the interfacial width depends on not only the orientation of the underlying solid but also the method used to determine the width. The widths based on the local order parameter, i.e., the difference between an actual local atomic configuration and a referential ideal crystalline one, are found to be able to reflect the transitions across the interface in both geometry and atomic motilities and are therefore reliable. These findings lay foundations for modelling the behavior related to the solid–liquid interfaces, such as the phase field simulation of crystal growth.

KEYWORDS: solid–liquid interface, molecular dynamics simulations, Cu–Ni alloy