ABSTRACT

Study of Morphological Instability of Kirkendall Voids by Phase-Field Simulations

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A quantitative multi-component phase-field model [1] is coupled with CALPHAD-type thermodynamic and kinetic databases to obtain a meso-scale description of Kirkendall void morphologies under isothermal annealing. The material under investigation is a diffusion couple consisting of a single-crystal Ni-based superalloy on one side and pure Ni on the other side. The flux of the fast diffuser Al towards the pure Ni causes a strong flux of vacancies in the opposite direction. This directed flux of vacancies leads to morphologically instable growth of voids, known as Mullins-Sekerka instability, in particular. Phase-field simulations are performed in two and three dimensions to fundamentally understand these instabilities by examining the effects of key kinetic parameters, such as the vacancy diffusion coefficient and vacancy source rate. It was shown that since these parameters differ at various distances from the diffusion couple interface, the size and shape of the voids can vary significantly, ranging from circular shapes to elongated dendrites. Additionally, asymmetrical shapes of voids can form due to interactions between neighboring voids.
In the experimental images obtained by synchrotron X-ray tomography, as well as in the simulations, we observed significant changes in void shapes along the diffusion couple. Near the Matano plane, the voids have elongated dendritic arms in the positive z-direction, whereas voids located at greater distances exhibit more symmetric dendritic forms or may even elongate in the opposite direction. Some voids resemble rounded pyramids, while others appear octahedral.

[1] J. Kundin, A. Riyahi khorasgani, R. Schiedung, B. Camin, I. Steinbach, Acta Materialia, 271, 119905 (2024).