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First-principles phase field method of microstructures in high-temperature alloys

E. Materials discovery, modeling, and characterization for sustainable energy applications

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Abstract

It is important to predict microstructures by computer simulation for effective design of high temperature alloys. However, since conventional phase field method has no ability of prediction because it uses empirical parameter to adjust to match experimental data. While first-principles calculations can not directly treat microstructures, whose typical length scale is 10μm. To overcome the problem, in this presentation, we will show the results of microstructure prediction of alloys by a first-principles phase field method (FPPF), which is originally developed by our research group [1]-[3]. In order to combine computational methods at different scales from nanoscale (first-principles calculations) to macroscale (phase field method), the potential renormalization theory and cluster expansion theory are used to obtain the free energy function as a step-wise function of the concentration φ_X of element *X*. Then solve the macroscale Cahn-Hilliard equation. We will show that the FPPF can predict microstructures of alloys such as Ni-Al alloy [1], Ti-6Al-4V alloy [2], Ti-Pt alloys and so on at high temperature region without any empirical parameter. For example, in the case of Ni-Al alloys at 1300K, the resulting patterns including cuboidal shaped precipitations are in excellent agreement with the experimental microstructures in each composition region of the Ni-Al phase diagram.

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