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A QUANTITATIVE FREE ENERGY FUNCTIONAL FOR PHASE FIELD MODELING

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It is often challenging to quantitatively predict the evolution of a microstructure in real-time and real-length scales during phase transformation using the phase field method. One of the major difficulties lies in constructing a physically sound and quantitative free energy functional for the system under investigation. This study attempts to quantify the chemical free energy density in the free energy functional for binary alloys that undergo phase transformation between disordered and ordered phases. A temperature dependent, quantitative free energy functional was developed for the modeling of hydride precipitation in zirconium alloys within phase field scheme. The model takes into account of crystallographic variants of hydrides, interfacial energy between hydride and matrix, interfacial energy between hydrides, elastoplastic hydride precipitation and interaction with externally applied stress. The model is fully quantitative in real time and real length scale, and simulation results were compared with limited experimental data available in the literature with a reasonable agreement. The work calls for experimental and/or theoretical investigations of some of the key material properties that are not yet available in the literature. This work was supported by a grant from Natural Science Foundation of China (51271157) and a grant from Research Grants Council of Hong Kong (PolyU 5267/10E).