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Total-spreading regime in phase-field modelling of microstructure evolution

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Abstract

Motivated by the beta-to-omega transformation in titanium alloys, the total-spreading regime is considered, in which two variants of the product (omega) phase cannot form a direct interface and are instead separated by a layer of the parent (beta) phase. For a relatively small thermodynamic driving force for transformation, this can be achieved by adopting the energy of the omega-omega interface to be higher than twice the energy of the beta-omega interface. For a large driving force, the ratio of the two interfacial energies must be sufficiently high to suppress the formation of direct interfaces between omega variants, which turns out to be challenging within the conventional multi-well phase-field framework. We discuss the limitations imposed by the requirements of algebraic and evolutionary consistency, as identified in [1]. To overcome these limitations, we propose an enhanced form of the algebraic part of the interfacial free-energy contribution, and a new mixing function in the chemical energy contribution [2]. As a side result, we provide a general and straightforward derivation of the constraints on the gradient part (capillary matrix) of the interfacial energy of constrained systems. Within the adopted framework, we can also easily show the equivalence of the diagonal and off-diagonal forms of the capillary and mobility matrices when the sum-to-unity constraint is enforced.

Keywords:

Interfaces Phase transition Total-spreading regime ω phase Titanium alloys Phase-field method

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