A variationally consistent and asymptotically convergent phase-field model for precipitation and dissolution

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Abstract

Available phase-field models for precipitation and dissolution (1, 2) are not variationally consistent, i.e. their governing equations are not derived starting from a free-energy functional, and do not incorporate nucleation. On the other hand, they fulfill the requirement that, as the regularization parameter tends to zero, convergence to an appropriate sharp-interface model is achieved. In this work, we develop a variational phase-field framework to model precipitation and dissolution. Our model features a closed-form expression of the free-energy functional, starting from which the non-linear coupled evolution equations of phase indicator and total ion concentration are obtained. The non-conserved phase indicator is assumed to be equal to the local solid volume fraction, and its evolution is governed by the Allen-Cahn equation. On the other hand, the conserved total ion concentration obeys the Cahn-Hilliard evolution law. In addition to being variationally consistent, our set of equations is also proved to converge to the appropriate sharp-interface model by applying the method of matched asymptotic expansions (3). The variational nature of our proposed model, beside offering a clearer physical interpretation and computational advantages, is also useful to incorporate nucleation of new precipitates, for which we propose a first possible approach.
References:

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