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Phase-field modeling of solute precipitation and dissolution at solid-fluid interface ZHIJIE XU, PAUL MEAKIN, Idaho National Laboratory — Phase phase-field methods have been developed to simulate a variety of processes in which interface dynamics play a critical role. The mathematical formulation of a phase field approach to the dynamics of liquid solid interfaces that evolve due to precipitation and/or dissolution will be presented. For the purpose of illustration, and comparison with other methods, phase field simulations have been carried out assuming first order reaction dissolution/precipitation) kinetics. In contrast to solidification processes controlled by a temperature field that is continuous at the solid/liquid interface, with a discontinuous temperature gradient, precipitation/dissolution is controlled by a solute concentration field that is discontinuous at the solid/liquid interface. The sharp-interface asymptotic analysis of the phase-field equations for solidification by Karma and Rappel [Phys. Rev. E57 (1998) 4342] have been extended to demonstrate that the phase-field equations converge to the proper sharp-interface limit for the precipitation/dissolution problem. The mathematical model has been validated for a one-dimensional precipitation/dissolution problem by comparison with the analytical solutions of the free-boundary problem.

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