

Computational Thermodynamics Models of Geomaterials Evolution using Phase Field

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We describe progress on the development of a new computational framework for grain-scale non-equilibrium thermodynamics for geomaterials problems. In our modeling approach, we couple the phase field equations for interfacial dynamics, chemical transport, and nucleation with thermodynamic and kinetic databases. Phase field techniques may be used to model grain coarsening, phase transformation, major and trace element diffusion, reactions, and the melting of minerals and rocks. We will describe the fundamental characteristics of such models, challenges in their development and interpretation, our efforts to adapt existing thermodynamic databases, provide examples for mantle systems and materials, and discuss future prospects for full integration into multiscale geodynamic models.