

Abstract Submitted
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Phase-field model and its numerical solution for coring and microstructure evolution studies in alloys¹ PATRICE E. A. TURCHI, JEAN-LUC FATTEBERT, MILO R. DORR, MICHAEL E. WICKETT, JAMES F. BELAK, Lawrence Livermore National Laboratory — We describe an algorithm for the numerical solution of a phase-field model (PFM) of microstructure evolution in alloys using physical parameters from thermodynamic (CALPHAD) and kinetic databases. The coupled system of PFM equations includes a local order parameter, a quaternion representation of local crystal orientation and a species composition parameter. Time evolution of microstructures and alloy composition is obtained using an implicit time integration of the system. Physical parameters in databases can be obtained either through experiment or first-principles calculations. Application to coring studies and microstructure evolution of Au-Ni will be presented.

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