



ICAMS Special Seminar

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Phase-field modeling of coring during solidification of alloy using quaternions and CALPHAD input

A numerical method for the simulation of microstructure evolution during the solidification of an alloy is presented. The approach is based on a phase-field model including a phase variable, an orientation variable given by a quaternion, the alloy composition, and a uniform temperature field. Energies and diffusion coefficients used in the model rely on thermodynamic and kinetic databases in the framework of the CALPHAD methodology. The numerical approach is based on a finite volume discretization and an implicit time-stepping algorithm. Its parallel implementation is based on the SAMRAI software infrastructure. Numerical results for solidification and accompanying coring effect in a Au-Ni alloy are used to illustrate the methodology.