

# Fully Coupled Thermodynamic/Kinetic Solution of Phase Transformations Under Non-Equilibrium Conditions

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## ABSTRACT

Boundary value problems involving a moving phase boundary ("Stefan Problems") are generally solved by making assumptions concerning the thermodynamic state of the interface – in the simplest case local thermodynamic equilibrium. For binary alloys and isothermal conditions, the problem is closed if the phase diagram is known, so that the kinetics of a phase transformation can be simulated [1]. For ternary alloys, the coupling of the diffusion of each alloying element needs to be considered, which is generally done by an iterative procedure equating the phase boundary velocities appearing in the mass balance of the alloying elements [2].

The situation becomes more complex if deviations from equilibrium at the phase boundary are considered. Early non-equilibrium phase transformation models used analytical equations that describe velocity dependent concentrations at the phase boundary [3]. The information from these equations replaces the phase diagram information, and the otherwise unchanged model can still be used. In the last decade, progress in describing the thermodynamic state at a phase boundary made full coupling of thermodynamics and kinetics of the phase transformation possible. Non-equilibrium thermodynamics requires that the total driving force for the phase transformation is subdivided into a part that actually drives the interface and a second part that accounts for the energy dissipation (for the adjustment of chemical potentials) inside the interface [4]. Both parts of the driving force come with their own mass balance equation, so that a simultaneous solution for the four coupled equations needs to be found. Depending on the type of phase transformation that is to be simulated (directional solidification with imposed velocity, equiaxed solidification from an undercooled melt, melting of a pure solid in a solute enriched liquid, etc.) the boundary conditions need to be defined which also define the given entities in the four equations. A solution for the unknown entities can then be found numerically.

Simulation results for different types of liquid/solid phase transformations (rapid growth of a solid nucleus [5], solutal melting, liquid film migration) are shown, demonstrating the versatility of the full solution of the coupled problem.

## REFERENCES

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