

## GRAND-CANONICAL FORMULATION OF PHASE-FIELD MODELS FOR ALLOY SOLIDIFICATION

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### EXTENDED ABSTRACT

The solidification of metallic alloys gives rise to the spontaneous formation of a large variety of different microstructures. This is a subject of fundamental interest as a well-controlled example of pattern formation, and of practical importance because of its applications in metallurgy [1]. These patterns arise from a subtle interplay between the destabilizing effects linked to the transport of heat and/or chemical constituents, and the stabilizing effect of interfacial properties such as capillarity and interface dissipation. In recent years, the phase-field technique has become the method of choice for the numerical modelling of solidification [2]. In its basic formulation, it can be obtained from Ginzburg-Landau free energy functionals through the standard phenomenological equations of out-of equilibrium thermodynamics that make use of variational principles. Its main advantage is that the explicit tracking of boundaries and interfaces is avoided by the introduction of scalar functions, the phase fields, which indicate the local state of matter and exhibit diffuse interfaces at phase boundaries. Moreover, this construction of the model implies that capillarity and interface dissipation are “automatically” contained in the equations.

For maximum computational efficiency, one would like to control independently the bulk and surface properties of the model. For alloy solidification, it can be shown that this is not the case in the formulations based on free-energy functionals [3; 4]. The basic underlying thermodynamic reason is that interface motion is controlled by the transport of an extensive quantity (chemical constituents), whereas interfacial equilibrium is controlled by the conjugate intensive quantities (the chemical potentials). Therefore, any model that describes the thermodynamics and transport phenomena in the bulk in terms of the extensive variables (compositions) makes the description of interface equilibrium (and the identification of the driving forces for interface motion) difficult. In contrast, a grand-canonical description in terms of the chemical potentials makes it easy to choose interpolation functions between the different phases that decouple bulk and interface properties [4]. In this formulation, the starting point is a grand-potential functional rather than a free-energy functional, and the dynamical variable is the local chemical potential. A complete analogy can be established between this formulation and the phase-field models for the solidification of a pure substance, which have traditionally used the temperature (the intensive quantity) as the dynamic variable. In this contribution, the formulation of the grand-canonical phase-field model for a binary alloy, its relation to the pure-substance model, and its extension to multi-component systems [5] will be discussed. Furthermore, a perspective for the construction of new phase-field models for other physical systems will be outlined.

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