

# A Thermodynamically-Consistent Phase Field Crystal Model of Solidification with Heat Flux

Cheng Wang<sup>1</sup> and Steven M. Wise<sup>2,\*</sup>

<sup>1</sup> *Department of Mathematics, The University of Massachusetts, North Dartmouth, MA 02747, USA ;*

<sup>2</sup> *Department of Mathematics, The University of Tennessee, Knoxville, TN 37996, USA.*

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**Abstract.** In this paper we describe a new model for solidification with heat flux using the phase field crystal (PFC) framework. The equations are thermodynamically consistent in the sense that the time rate of change of the entropy density is positive in the bulk and at the boundaries of the domain of interest. The resulting model consists of two equations, a heat-like equation and a mass-conservation equation that describes how the atom density changes in time and space. The model is simple, yet it can properly capture the variation in the free energy landscape as the temperature is changed. We describe the procedure for constructing a temperature-atom-density phase diagram using this energy landscape, and we give a simple demonstration of solidification using the model.

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## 1 Introduction

The phase field crystal (PFC) model was introduced in [13, 14] as continuum description of solidification in a unary material. It was formulated as a mass conservative version of the classical Swift-Hohenberg equation, but, later, the model was re-derived, via certain reasonable simplifications, from the dynamical density functional theory (DDFT) [15]. In particular, assuming a constant, uniform temperature field  $T$ , one expresses the Helmholtz free energy density via

$$F = \int_{\Omega} \left\{ f(T, \rho) + \frac{T\kappa_{f,\rho,\rho}}{2} (\rho - \rho_0) \mathcal{C}(\rho - \rho_0) \right\} dx,$$

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\*Corresponding author. *Email addresses:* cwang1@umassd.edu (Wang C), swise1@utk.edu (Wise S M)

where  $\Omega$  is some spatial domain of interest,  $\rho : \Omega \rightarrow [0, \infty)$  is the number density field of the unary material in  $\Omega$ , the constant  $\rho_0 > 0$  is a reference density,  $\kappa_{f,\rho,\rho} > 0$  is a positive constant,  $f$  is the homogeneous Helmholtz free energy density, and  $\mathcal{C}$  is a symmetric, potentially nonlocal, two-point correlation operator. The free energy density,  $f$ , is often taken to satisfy an ideal “gas” model:

$$f(T, \rho) = \rho k_B T \ln \left( \frac{\rho}{\rho_0} \right) - k_B T (\rho - \rho_0),$$

where  $k_B$  is the Boltzmann constant. Often, one makes a (Taylor) polynomial approximation of the logarithmic term about the reference density to make the model more tractable. However, it is the singular nature of the logarithmic term that guarantees the positivity of the solutions, and this is an important feature in the numerical and PDE analyses. At constant temperature, one can argue that the dynamics of the model should satisfy a diffusion-dominated mass conservation equation of the form

$$\dot{\rho} = -\nabla \cdot \mathbf{J}, \quad \mathbf{J} = -M\rho \nabla \mu, \quad (1.1)$$

where  $\mathbf{J}$  is the diffusion flux,  $M > 0$  is a mobility, and  $\mu$  is the chemical potential:

$$\mu := \delta_\rho F = k_B T \log(\rho) + T \kappa_{f,\rho,\rho} \mathcal{C}(\rho - \rho_0), \quad (1.2)$$

where we have assumed, for simplicity, that the boundary conditions are periodic. As a consequence of these assumptions, the total free energy is dissipated as the system evolves toward equilibrium, and the dissipation rate is

$$\dot{F} = -M \int_{\Omega} \rho |\nabla \mu|^2 dx \leq 0.$$

Of course, it would be necessary to justify the property that  $\rho > 0$  (or at least  $\rho \geq 0$ ) pointwise for the model to make sense. Numerical analyses of similar gradient flow models, that is, models that have logarithmic energy potentials, have been performed in [5, 10–12, 19, 20, 23, 28].

The PFC modeling framework has a couple of basic, distinctive features. First, the solutions to the PFC-type models exhibit (at least) two distinct phases. One is a spatially oscillatory phase, which is identified with the solid phase, and the other is a spatially uniform phase, which is usually identified as the liquid (or gas) phase. The peaks of the solutions in the oscillatory phase are interpreted as the “locations” of the atoms, and typically, one can choose  $\mathcal{C}$  so that the peaks are arranged in a desired crystal structure [21]. Second, PFC models operate at atomic length scales but diffusive time scales. Thus, the framework can capture long-time phenomena.

In this paper, we will devise a new model for solidification and melting using the phase field crystal framework. In particular, we will not assume that the temperature is uniform in space and time. For an adiabatically isolated system, this requires that the