Physica D 308 (2015) 1–10

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Traveling wave profiles for a crystalline front invading liquid states: Analytical and numerical solutions

P.K. Galenko [a,b,*], F. Iunes Sanches [c], K.R. Elder [c]

[a] *Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, D-07743 Jena, Germany*

[b] *Ural Federal University, Laboratory of Multi-Scale Mathematical Modeling, 620002 Ekaterinburg, Russia*

[c] *Department of Physics, Oakland University, Rochester, MI, 48309-4487, USA*

HIGHLIGHTS

- Manuscript provides analytic solution for traveling wave profiles of the phase field crystal model in two dimensions.
- Solutions are derived for both parabolic and hyperbolic cases for a crystalline state invading both metastable and unstable liquids.
- Solutions are verified numerically and shown to be accurate in the small velocity limit near the liquid/solid phase transition.

ARTICLE INFO

Article history:
Received 13 January 2014
Received in revised form
3 January 2015
Accepted 1 June 2015
Available online 9 June 2015
Communicated by J. Dawes

Keywords:
Crystal
Model
Pattern selection
Traveling wave

ABSTRACT

The properties of a two dimensional crystalline phase invading a metastable or unstable liquid state are examined using the amplitude expansion formulation of the hyperbolic and parabolic phase-field crystal model. When the amplitudes are real and equal to each other, analytic expressions are derived for the profile of a steady state liquid–solid front traveling at constant velocity. Numerical simulations of the full amplitude formulation are conducted and compared with the analytic results. Close to the melting transition the analytic results for the liquid–solid profile, velocity and width are in quantitative agreement with the numerical results and disagree far from the transition.

1. Introduction

When phase transformations occur it is often the case that interfaces or domain walls form between different phases or states. The interaction and motion of these interfaces play a key role in the subsequent evolution of the system. For example, in order–disorder transitions domain walls form between different, but energetically equivalent, variants of a given sublattice ordering. Subsequent evolution towards equilibrium is then thought to be driven by the curvature of the domain walls [1]. One reason that many studies [2–4] have been devoted to understand the dynamics and motion of such domain walls is that the motion often leads to complex spatial structures which strongly influence material properties. For example, properties such as the yield strength and magnetic coercivity are known to be a strong function of grain size in polycrystalline materials [5]. Another interesting aspect of interface motion is that when a stable phase invades a metastable or unstable phase it is possible that the state that is selected at the front is not exactly the equilibrium state as occurs when a periodic phase invades a uniform state. In this instance, the periodicity that is selected near the propagating front may not be the equilibrium periodicity. This could potentially lead to a strained state or in extreme circumstances a glassy state [6].

Recently, the phase field crystal (PFC) model has been used to examine the dynamics of liquid–solid, grain boundaries and dislocation motion [7–10]. The PFC model is a continuum model that describes processes on atomic length scales and patterns on the nano- and micro-length scales [10,11]. This model is characterized by a free energy that is a functional of a field (n) that is periodic in the solid phase and uniform in a liquid state and an equation of motion that conserves the average value of n. The periodicity of n naturally incorporates elasticity and multiple crystal orientation which allows the model to be used to study a number of phenomena including epitaxial growth, ordering of nano-scale

---

[*] Corresponding author at: Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, D-07743 Jena, Germany.

E-mail address: peter.galenko@uni-jena.de (P.K. Galenko).

http://dx.doi.org/10.1016/j.physd.2015.06.002
0167-2789/

structures on micron length scales [11], liquid–solid transitions, dislocation motion and plasticity, glass formation and foams, grain boundary premelting, crack propagation, surface reconstructions, grain boundary energies, dynamics of colloidal systems and polymers (see overview [12] and references therein).

In a previous work the selection of a periodic state as it invades an unstable state was examined in the one-dimensional PFC-model with both hyperbolic and parabolic dynamics [6]. A marginal stability analysis was used to determine the velocity and periodicity of the front. It was found that the periodicity of the selected state was different from the equilibrium state and as expected did depend on the type of dynamics. For very high driving forces it was also found that the periodicity selected was above the Eckhaus instability leading to the speculation of glassy states. The results of the work [6] were quantitatively verified with direct numerical simulations [13].

In this work we consider the solidification of a crystalline state from a metastable or unstable liquid state as described by the two-dimensional PFC model and develop analytic solutions for a crystalline front invading the liquid. Here we assume that the transition from the metastable state to the stable state occurs by overcoming the energy barrier which is usually necessary for the emergence of a new phase. Contrary to that, the transition from the unstable state proceeds without energetic barrier that is usually evolves by fluctuation mechanism. The analysis of these two transitions is based on the amplitude representation of the PFC model [14,15] in which the conserved scalar field n is represented by a set of complex amplitudes that are assumed to vary on length scales larger than the wavelength of n. The phase of the amplitudes allows for elastic strains and multiple crystal orientation and the magnitude of the amplitudes incorporates liquid–solid interfaces and transitions. The combination of the phase and magnitude allows for more complex features such as dislocations and grain boundaries. However, some features, such as Peierls barriers and faceting are missing from the amplitude description used in this work, although higher order corrections are possible [16]. In this paper analytic solutions for a crystalline front invading an unstable and metastable liquid state are derived in the limit in which the amplitude can be represented by a single magnitude only. For comparison, numerical simulations of the full amplitude description are also conducted.

The paper is organized as follows. Section 2 presents a formulation of the model which introduces governing hyperbolic PFC-equation. This equation describes simultaneously dissipation for diffusive regimes existing in slow transitions and inertia for propagative regimes occurring in fast phase transitions. In Section 3, the amplitude equations are first introduced and then simplified to a magnitude (ϕ) only description. In Section 4 the equilibrium properties of the system are described in terms of ϕ. The dynamics and traveling wave solution for the real amplitude of the triangular pattern propagating into unstable and metastable homogeneous states are obtained. In Section 5, numerical solutions of the full amplitude formalism are presented and compared with the analytic solutions. Conclusions are given in Section 6. Appendix A presents details of analytical method based on amplitude wave representation. Appendix B gives details of the computational scheme used in the numerical modeling. Finally, Appendix C describes numerical estimations for the relaxation times used in the presented model.

2. Hyperbolic PFC-model

The hyperbolic PFC model describes a first order liquid–solid transformation in terms of a field, $n(\vec{r},t)$, that is related to the dimensionless local atomic number density and a flux $\vec{J}(\vec{r},t)$. The free energy functional [6,17] is a functional of n and $\vec{J}$ and can be written in dimensionless form as

$$\mathcal{F}[n,\vec{J}] = \mathcal{F}_{eq}[n] + \mathcal{F}_{neq}[\vec{J}]. \tag{1}$$

The local equilibrium contribution is given by [18]

$$\mathcal{F}_{eq} = \int \left[\frac{n}{2}\mathcal{L}\,n - \frac{a}{3}n^3 + \frac{v}{4}n^4\right] d\vec{r}, \tag{2}$$

where

$$\mathcal{L} \equiv \Delta B_0 + B_0^x(1+2R_o^2\nabla^2)^2. \tag{3}$$

ΔB_0, B_0^x, R_o, a and v are phenomenological parameters that can be fit to various physical properties of the systems as discussed in references [19,20,18,21]. Briefly the sum, $B_0^\ell = \Delta B_0 + B_0^x$, is the dimensionless liquid state compressibility, B_0^x is proportional to the elastic moduli, R_o sets the length scale of the lattice and a and v determine the magnitude of the fluctuations in the solid state and the size of the miscibility gap in n at liquid–solid coexistence. The free energy functional (2) describes a transition from a liquid state (n = constant) at high ΔB_0 to a crystalline state (n = periodic) at low or negative values of ΔB_0 [18,21]. In this respect, the parameter ΔB_0 can be thought of as a control parameter similar to a temperature difference.

The nonequilibrium contribution is given by

$$\mathcal{F}_{neq}[\vec{J}] = \frac{\tau}{2}\int \vec{J}\cdot\vec{J}\,d\vec{r}, \qquad \tau > 0, \tag{4}$$

where τ is the characteristic time for relaxation of the flux $\vec{J}$ to its steady state. The dynamics are described by a continuity equation to ensure conservation of n, i.e.,

$$\frac{\partial n}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0. \tag{5}$$

The non-equilibrium contribution to energy (4) is introduced phenomenologically by the extended thermodynamics [22] or by the generalized hydrodynamics [23]. The requirement that the free energy given in Eq. (1) decreases (or is constant) in time leads to the hyperbolic equation [17,24]:

$$\tau\frac{\partial^2 n}{\partial t^2} + \frac{\partial n}{\partial t} = \nabla^2\left[\mathcal{L}n - an^2 + vn^3\right]. \tag{6}$$

The hyperbolic phase-field equation (6) contains both the relaxation of slow conserved variable $n(\vec{r},t)$ and fast non-conserved variable $\vec{J}(\vec{r},t)$ to their own steady-states (see Ref. [22] and references therein). As a result of these two relaxation processes, Eq. (6) shows that, in addition to the dissipation described by the traditional parabolic PFC-equation [7], inertia $\propto \partial^2 n/\partial t^2$ is also taken into account due to kinetic contribution (4). Alternatively, Eq. (6) was proposed by Stefanovic et al. [25,26] to incorporate both fast elastic relaxation and slower mass diffusion. Similar equations have also been obtained using dynamical density functional theory by Archer [27]. As a result, Eq. (6) can describe the dynamics of a periodic crystalline state invading a metastable or unstable liquid state and vice versa. To obtain an understanding of these processes an analytic solution will be derived by considering an amplitude representation of Eq. (6) as described in the next section.

3. Amplitude's equation

For mathematical convenience it is useful to write the solutions of the atomic density n in terms of the following expansion

$$\begin{aligned} n &= n_o + \sum_{klm}\eta_{klm}\exp\left(i\vec{G}_{klm}\cdot\vec{r}\right) + \sum_{klm}\eta^*_{klm}\exp\left(-i\vec{G}_{klm}\cdot\vec{r}\right) \\ &\equiv n_o + \sum_{j=1}^{3}\left[\eta_{klm}\exp\left(i\vec{G}_{klm}\cdot\vec{r}\right) + \text{c.c.}\right], \end{aligned} \tag{7}$$