



# A modified two-mode phase-field crystal model applied to face-centered cubic and body-centered cubic orderings



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## ARTICLE INFO

### Article history:

Received 9 March 2015

Accepted 6 April 2015

Available online 5 May 2015

### Keywords:

Phase-field crystals

Solid–liquid

Nano-structure

## ABSTRACT

In this work, we present a modified two-mode phase-field crystal (PFC) model for nano-structural evolution of materials. The model is used to study both the face-centered cubic (FCC) and body-centered cubic (BCC) orderings, as well as the solid–liquid coexisting phenomenon. This two-mode PFC model incorporates three parameters in its formulation and damps out the dynamics of the system, except near the first two critical wavelengths. The material properties such as volume expansion and free energy change in melting, crystalline structure, solid density wave amplitudes, and elastic constants can be determined by this PFC model.

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Phase-field crystal (PFC) is an atomistic model acting on diffusive time scales [1,2], which naturally incorporates different physical phenomena such as elasticity, two-phase interfaces, vacancies, and grain boundaries in its formulation [3–6]. Thus, PFC is of great interest in studying structures and properties of metallic materials. The original PFC model was a reformulation of the conserved version of the Swift–Hohenberg (SH) equation for thermal fluctuations in Rayleigh–Benard convection problem [7,8]. The free energy of the original PFC model is [1,7]

$$F = \int_V \left\{ \frac{1}{2} \psi [-\varepsilon + (1 + \nabla^2)^2] \psi + \frac{\psi^4}{4} \right\} d\vec{r} \quad (1)$$

where  $\psi(\vec{r}, t)$  is the dimensionless density field,  $\vec{r}$  is the position vector,  $t$  is the time, and  $\varepsilon$  is a model parameter. In the concept of density functional theory (DFT), the density of the crystalline state can be expressed in terms of the reciprocal lattice vectors (RLVs),  $\vec{k}$ , by

$$\psi = \psi_s + \sum_{\vec{k}} A_{\vec{k}} e^{i\vec{k} \cdot \vec{r}}. \quad (2)$$

In Eq. (2),  $\psi_s$  is the average density in the solid state, and  $A_{\vec{k}}$  is the Fourier amplitudes of the related RLVs. The PFC free energy in Eq. (1) only uses the first set of RLVs (one-mode PFC model). Therefore, it can represent (by only minimizing the free energy) principal RLVs with closed triangle forms, which are hexagonal and BCC structures in two-dimensional (2D) and three-dimensional (3D) spaces, respectively [9]. The one-mode PFC model is already applied to study

different phenomena in materials science, including solidification [10], elastic deformation [11], spinoidal decomposition [12], grain boundary premelting [13], dislocation dynamics [14], and Kirkendall effect [15]. Furthermore, it was shown that the one-mode PFC model can be used to quantitatively simulate the two-phase solid–liquid coexistence of Fe [16–18] by determining its model parameters from molecular dynamics (MD) simulations. For most of the above mentioned applications of the one-mode PFC model, the crystalline state is hexagonal in 2D and BCC in 3D.

Theoretically, it is possible to stabilize other lattice orderings by including more RLVs in Eqs. (1) and (2). Wu et al. [9] presented a two-mode PFC model by modifying the two-frequency SH equation, which was introduced by Lifshitz and Petrich [19]. Their two-mode PFC model uses first two sets of RLVs and shows square and FCC orderings in 2D and 3D, respectively. Wu et al. [9] also presented a method to determine the two-mode PFC model parameters for Ni from the results of MD simulations. The capability of their model in quantitative calculations of the two-phase solid–liquid coexistence properties, such as interface free energy and expansion in melting, is yet to be known. A PFC model for BCC–liquid coexistence was presented by Jaatinen et al. [20] which is of eight-order in spatial derivatives (EOF-PFC). The EOF-PFC model was also used to quantitatively study the solid–liquid coexistence of Fe [20] and it was used to study 2D crystallization as well [21]. Greenwood et al. [22–24] developed a class of two-mode PFC models which are also suitable to model structural phase transformations in metals by using Gaussian distribution function to approximate the solid density waves. Recently, Mkhonta et al. [25] presented a multimode PFC model in 2D, which was inspired by the work of Wu and coworkers. They argued that including first

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three sets of RLVs (three-mode PFC) in the PFC model is sufficient to form all the five Bravais lattices and many non-Bravais structures such as honeycomb and kagome phases.

In this work, we present a modified two-mode PFC model that shows both FCC and BCC orderings in 3D, as well as their coexistence with the liquid state. The present PFC model includes first two RLVs in Eqs. (1) and (2), but it (similar to the model of Wu et al. [9]) has three parameters that can be used to adjust the relative solid–liquid free energies and densities, as well as the relative Fourier amplitudes of the first two RLVs. We also present the phase diagrams for the FCC–liquid and BCC–liquid coexistence as functions of these model parameters.

For FCC and BCC lattices, the first principal RLV is related to  $[111]$  and  $[110]$  density wave vectors ( $\vec{k}_{111}$  and  $\vec{k}_{110}$ ), respectively. Although in theory there is freedom in the selection of the second density wave vector, it is more advantageous computationally to choose the second wavelength as close as possible to the first wavelength. Thus, we choose the second RLV for both FCC and BCC crystals to be  $[200]$  density wave vector ( $\vec{k}_{200}$ ). We propose the following Helmholtz free energy for the two-mode PFC model

$$F = \int_V \left\{ \frac{\psi}{2} \left[ -\varepsilon + [(1 + \nabla^2)^2 + R_0] \left[ (Q_1^2 + \nabla^2)^2 + R_1 \right] \right] \psi + \frac{\psi^4}{4} \right\} d\vec{r}, \quad (3)$$

where  $\varepsilon$  is an adjustable small positive parameter,  $R_1$  is the second adjustable small parameter which can be positive or negative, and  $R_0$  is a parameter which will be determined as a function of  $R_1$  and the Fourier amplitudes of the RLVs. In Eq. (3),  $Q_1$  is the ratio of the second wavelength to the first wavelength for the considered lattice structure; i.e.,  $Q_1 = |\vec{k}_{200}| / |\vec{k}_{111}| = \sqrt{4/3}$  for FCC, and  $Q_1 = |\vec{k}_{200}| / |\vec{k}_{110}| = \sqrt{2}$  for BCC. This two-mode PFC model maybe used for other type of lattice structures in 3D, such as HCP and diamond, and in 2D, such as square lattices. Exploring the capability of this two-mode PFC model for simulating other lattice structures requires further study of this model, which will be presented in the future works.

In order to explore the capabilities of the two-mode PFC in modeling solid–liquid equilibrium, the free energy for the liquid and crystalline states must be calculated in terms of the model parameters:  $\varepsilon$ ,  $R_1$  and  $R_0$ . Thus, we first present the relations for the density field in the crystalline states. We denote the Fourier amplitudes of the first and second RLVs by  $A_i$  and  $B_i$ , respectively. Assuming the same amplitudes for all the density waves in the solid state ( $|A_i| = A_s$  and  $|B_i| = B_s$ ), the density field in the solid state for FCC and BCC crystals, following Eq. (2), become

$$\psi_{fcc} = \psi_s + 8A_s \cos qx \cos qy \cos qz + 2B_s (\cos 2qx + \cos 2qy + \cos 2qz), \quad (4a)$$

$$\psi_{bcc} = \psi_s + 4A_s (\cos qx \cos qy + \cos qx \cos qz + \cos qy \cos qz) + 2B_s (\cos 2qx + \cos 2qy + \cos 2qz), \quad (4b)$$

where  $q = 1/\sqrt{3}$  for FCC and  $q = 1/\sqrt{2}$  for BCC. The free energy density in the solid state,  $f_{fcc}$  or  $f_{bcc}$ , is obtained by substituting Eq. (4) into Eq. (3), integrating over a lattice cell, and dividing the resultants by the volume of the lattice cell:

$$\begin{aligned} f_{fcc} = & - \left[ \varepsilon - (1 + R_0) \left( \frac{16}{9} + R_1 \right) \right] \frac{\psi_s^2}{2} + \frac{\psi_s^4}{4} \\ & + 4 \left( \frac{1}{9} R_0 - \varepsilon + R_0 R_1 + 3\psi_s^2 \right) A_s^2 \\ & + 3 \left( 3\psi_s^2 + R_0 R_1 + \frac{1}{9} R_1 - \varepsilon \right) B_s^2 + 72A_s^2 B_s \psi_s + 144A_s^2 B_s^2 \\ & + 54A_s^4 + \frac{45}{2} B_s^4, \end{aligned} \quad (5a)$$

$$\begin{aligned} f_{bcc} = & - [\varepsilon - (1 + R_0)(4 + R_1)] \frac{\psi_s^2}{2} + \frac{\psi_s^4}{4} \\ & + 6(R_0 - \varepsilon + R_0 R_1 + 3\psi_s^2) A_s^2 \\ & + 3(3\psi_s^2 + R_0 R_1 + R_1 - \varepsilon) B_s^2 + 72A_s^2 B_s \psi_s + 144A_s^2 B_s^2 \\ & + 144A_s^3 B_s + 48A_s^3 \psi_s + 135A_s^4 + \frac{45}{2} B_s^4. \end{aligned} \quad (5b)$$

By minimizing the above free energy densities with respect to  $q$ , we obtain  $R_0 = R_1 (B_s^2/A_s^2)$ . It is worth mentioning that the present two-mode PFC model recovers the two-mode PFC model of Wu et al. [9] if  $R_0 = 0$ . However, if  $R_0 = 0$ , the total free energy is not minimized with respect to  $q$ , unless  $R_1 = 0$ ; i.e.,  $df_{fcc}/dq|_{q=1/\sqrt{3}} = 16B_s^2 R_1/\sqrt{3}$  and  $df_{bcc}/dq|_{q=1/2} = 48B_s^2 R_1/\sqrt{2}$ . As it might be clear, this error in minimization of the total free energy increases as  $R_1$  or  $B_s$  increases. Therefore, inclusion of  $R_0$  in two-mode PFC models is necessary to avoid error in the minimization of the free energy in the crystalline state. In addition, by substitution of  $R_1 = 0$  in Eq. (3), the present two-mode PFC model becomes the two-frequency SH model introduced by Lifshitz and Petrich [19]. In later stages of this paper, it will be shown that the inclusion of  $R_1$  in the formulation gives the freedom to vary properties such as expansion and free energy changes in melting, as well as the relative amplitudes of the RLVs.

Further minimization of  $f_{fcc}$  and  $f_{bcc}$  with respect to  $A_s$  and  $B_s$  results in relations for determining the density amplitudes of FCC and BCC crystals in terms of  $\psi_s$ ,  $R_1$  and  $\varepsilon$ ; these relations are not presented here for brevity.

The free energy density in the liquid phase,  $f_l$ , is obtained by substituting the constant liquid density,  $\psi_l$ , in Eq. (3), integrating over a lattice cell, and dividing the resultant by the volume of the lattice cell:

$$f_l = - \left[ \varepsilon - (1 + R_0)(Q_1^4 + R_1) \right] \frac{\psi_l^2}{2} + \frac{\psi_l^4}{4}. \quad (6)$$

The only unknowns left in the model are the coexistence average densities,  $\psi_l$  and  $\psi_s$ , which are related to  $\varepsilon$  and  $R_1$ , and can be obtained by the construction of the standard common tangent line for solid and liquid free energies in Eqs. (5) and (6). This task is done numerically.

The phase diagrams of FCC–liquid and BCC–liquid coexistence for different  $R_1$  parameters are plotted in Fig. 1(a) and (b), respectively. To show the effect of  $R_1$  parameter on the phase diagrams, three different values are chosen for the  $R_1$  parameter;  $R_1$  is either zero, a positive value or a negative value. Change in  $R_1$  has a stronger effect on the phase diagram of BCC–liquid coexistence, especially for a negative value of  $R_1$ . Thus, the phase diagrams are presented for the choices of  $R_1 = -0.01$  and  $R_1 = -0.1$  for BCC and FCC crystals, respectively. Theoretically, the parameter  $R_1$  can be increased to big positive or negative values. However, as  $R_1$  increases to a big positive (negative) value, the effect of the second wave vector decreases (increases) severely, such that the Fourier amplitude of the second (first) wave vector,  $B_s(A_s)$ , vanishes. For a typical FCC or BCC crystal,  $B_s/A_s$  is a positive number less than one; so the choice of  $R_1$  in the model is practically limited to small values in order to represent real FCC and BCC crystals, and to avoid computational deficiency in the model (by introducing zero  $A_s$  or  $B_s$ ).

The values of expansion in melting,  $\Delta\psi = \psi_l - \psi_s$ , for  $\varepsilon = 0.042$  are also shown in Fig. 1. It is interesting to note that increasing  $R_1$  parameter from zero to positive values shifts the coexisting lines toward smaller densities and decreases the expansion in melting, and decreasing  $R_1$  parameter from zero to negative values has reverse effects. To clearly illustrate the coexistence of solid and liquid in the presented two-mode PFC model, the free energy

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