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A quantitative phase-field model for two-phase elastically inhomogeneous systems

A. Durga *, P. Wollants, N. Moelans

Department of Materials Engineering, Faculty of Engineering, KU Leuven, Kasteelpark Arenberg 44 Bus 2450, BE-3001 Leuven, Belgium

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ABSTRACT

Solid-state phase transformations are influenced by strains that are generated internally or applied externally. The stress state, composition, and microstructure evolution, which together determine the properties of solid materials can be studied using phase-field models coupled with micro-elasticity theory in the small strain limit. This coupling has been implemented using various schemes in literature. In a previous article (Durga et al., 2013), the authors evaluated three main existing schemes for a two-phase system and concluded that these schemes are not quantitative for inhomogeneous anisotropic elastic properties of the two phases. The stress states predicted by these models deviate from the expected values due to the generation of extra interfacial energy, which is an artefact of the models resulting from interfacial conditions different from local mechanical equilibrium conditions. In this work, we propose a new scheme with interfacial conditions consistent with those of the analytical results applicable to a general system where shear strains may be present. Using analytical solutions for composition and stress evolution, we validate this model for 2D and 3D systems with planar interface in the presence of misfit between phases and applied strains, and a 2D system with an elliptical second-phase particle. This extended scheme can now be applied to simulate quantitatively the microstructural evolution with coupled chemical and mechanical behaviour in any 2D or 3D two-phase system subject to internal or external strains irrespective of interface curvature.

1. Introduction

Phase-field models are used to solve moving boundary problems such as phase transformations in solid and liquid states and transport phenomena involving fluid flow or mass diffusion, which involve elastic, magnetic, electrochemical and other physical effects. The main advantage of this method is the use of a diffuse interface between different domains. This is represented by one or more phase-field variables which vary continuously across the interface. The evolution of the system is then driven by the minimisation of total free energy, which is a function of the phase-field variables in space and time. In this article, a quantitative phase-field model considering the effects of chemical diffusion and linear elasticity on microstructure evolution in solid-state materials is presented.

Phase-field models coupled with microelasticity theory have been extensively applied to study various phenomena such as martensite transformations [2], grain growth, and texture evolution [3]. Several schemes are available in literature that combine micro-elasticity theory with phase-field models. Steinbach-Apel's scheme (SAS) [4], Voigt-Taylor's scheme (VTS) [5,6], and Khachaturyan's scheme (KHS) [7] are the three main existing schemes. They differ in the way the elastic strain, stress, and elastic constants are defined in the diffuse interface, which in turn causes a difference in the elastic contribution to the driving force for the system evolution. There have been only limited [4,5,8] comparative studies of these schemes with analytical solutions, especially for complex morphologies of inhomogeneous systems and the coupling with chemical equilibrium.

In 'thin interface' phase-field models [9], the interface width is generally taken abnormally large compared to the actual physical interface width in materials. In order to provide reliable results, we need to use quantitative models, i.e. those that do not depend on the value of the diffuse interface width used in the phase-field model. The results have to be independent of the value of the interface width as long as the microstructural features of interest are larger than the interface width. Such quantitative phase-field models are available for studying phase transformations and diffusion in multiphase systems [10], solidification [11] and grain growth [12]. These models ensure that the bulk energy of the system is

* Corresponding author. Tel.: +32 16 373734.
E-mail addresses: durga87@gmail.com (A. Durga), patrick.wollants@mtm.kuleuven.be (P. Wollants), nele.moelans@mtm.kuleuven.be (N. Moelans).

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decoupled from the interfacial energy that arises due to the diffuse interface. Coupling phase-field models with elasticity, however, presents a complication due to the presence of many inter-related tensorial quantities such as the elastic strain, the elastic stress, stiffness, and the displacement fields. Therefore, a simple analogy with the other quantitative models does not exist. Examples of quantitative phase-field models with tensorial fields include that of Nicoli et al. [13], which uses mobility tensor for a two-phase system with different interpolations for different components of the tensor, and Yeon et al. [8], wherein a quantitative elastic phase-field model for binary coherent two-phase systems with stiffnesses of cubic symmetry is presented.

In a previous work [1], the authors studied a two-phase inhomogeneous system separated by a planar interface and showed that the interpolation of elastic properties in phase-field models following the schemes of KHS, SAS, and VTS are not quantitative, i.e., the bulk properties depend on the diffuse interface width used in the model and excess interfacial energy is created due to the elastic energy formulation. The three schemes are quantitative only under special circumstances: KHS when the elastic strains are equal in the two phases, SAS when the stresses are equal in the two phases and VTS when the total strains are equal in the two phases. We then introduced a new quantitative scheme which uses interfacial conditions that are consistent with the analytical results. We validated this scheme for a 2-D two-phase system with a planar interface in the absence of shear strains. However, in order to be applicable to a general two-phase system with arbitrary interface curvatures and shear strains in 2-D and 3-D, the model needs to be further developed and validated.

The aim of this work is to extend and validate the new scheme for 2D and 3D two-phase systems with shear strains, arbitrary interface curvature, and no restriction on the nature of the elastic constants. The model is validated for the following cases of two-phase systems using corresponding analytical solutions: (i) planar interface with shear strains and applied strains in 2D and 3D (Johnson's analytical model [14]) and (ii) elliptical precipitate in a large matrix in 2D (Jin et al.'s analytical solution [15]).

The rest of the paper is organised as follows. First, we discuss analytical solutions available for 2D and 3D systems in Section 2. Then, the phase-field model used in this study is given in Section 3. The coupling of elastic energy with the phase-field model using the new quantitative scheme is formulated in Section 4. Section 5 discusses the simulation results for the different cases and the main conclusions are drawn in Section 6.

2. Analytical solutions

Starting with a brief introduction to microelasticity theory, we present analytical solutions available in the literature for 3 cases: Johnson's description [14] for 2D and 3D systems with planar interface, and Jin et al.'s solution [15] for a 2D system with an elliptical second-phase precipitate. These will be compared with results from the phase-field simulations in order to validate the model.

2.1. Microelasticity theory

We consider a coherent two-phase system. No assumptions are made about the nature of the elastic moduli. Undeformed α phase is taken as the reference state for the calculation of eigenstrain. The stresses and strains are defined in the system according to Khachaturyan [7]. The elastic stress in the small-strain regime, where linear elasticity theory holds, is given by:

$$\sigma_{ij} = C_{ijkl}\epsilon^{el}_{kl}, \tag{1}$$

where C_{ijkl} is the stiffness tensor and ϵ^{el}_{kl} the elastic strain. Einstein summation notation is used for all equations involving tensors in this article.

Elastic strain is defined as:

$$\epsilon^{el}_{kl} = \epsilon_{kl} - \epsilon^{*}_{kl} = \overline{\epsilon_{kl}} + \delta\epsilon_{kl} - \epsilon^{*}_{kl}, \tag{2}$$

where $\epsilon_{kl} = \overline{\epsilon_{kl}} + \delta\epsilon_{kl}$ is the total strain. ϵ^{*}_{kl} is the eigenstrain given by the relative difference in the lattice parameters of the two phases. Taking underformed α as the reference state, the eigenstrains are then zero in the α phase and typically non-zero in the β phase. $\overline{\epsilon_{kl}}$ is the homogeneous or applied strain defined such that

$$\int_V \delta\epsilon_{kl} d^3r = 0. \tag{3}$$

The heterogeneous strain $\delta\epsilon_{kl}$ is related to the local displacement fields $u_i(\vec{r})$ as

$$\delta\epsilon_{kl} = \frac{1}{2}\left[\frac{\partial u_k(\vec{r})}{\partial r_l} + \frac{\partial u_l(\vec{r})}{\partial r_k}\right]. \tag{4}$$

The elastic energy density is then given by:

$$f^{el} = \frac{1}{2}\epsilon^{el}_{ij} C_{ijkl} \epsilon^{el}_{kl}. \tag{5}$$

At mechanical equilibrium, $\frac{\partial \sigma_{ij}}{\partial r_j} = 0$.

2.2. Johnson's model

Johnson's description gives the conditions for interfacial mechanical and chemical equilibrium. In Sections 2.2.1 and 2.2.2, the mechanical equilibrium is given for 2D and 3D systems with planar interfaces respectively. In Section 2.2.3, the equilibrium compositions in the presence of strains is given, which can be calculated on knowing the stress state of the system.

2.2.1. 2D system with misfit between phases and applied strains

Considering a 2D rectangular two-phase system as shown in Fig. 1(a), the equilibrium interfacial relations for the stresses and strains are as follows. There is continuity of displacements and tractions at the interface:

$$u^{\alpha}_i = u^{\beta}_i, \tag{6}$$

$$\sigma^{\alpha}_{ij} n^{\alpha}_j + \sigma^{\beta}_{ij} n^{\beta}_j = 0, \tag{7}$$

where n_j are the components of the outward pointing unit normals to the respective phases at the interface. From the geometry, $n^{\alpha}_1 = -n^{\beta}_1$ and $n^{\alpha}_2 = n^{\beta}_2 = 0$. For $i = 1$, (7) gives $\sigma^{\alpha}_{11} = \sigma^{\beta}_{11}$, and for $i = 2$, $\sigma^{\alpha}_{12} = \sigma^{\beta}_{12}$. Expanding these two equalities, we get

$$\begin{aligned} &C^{\alpha}_{1111}(\bar{\epsilon}_{11} + \delta\epsilon^{\alpha}_{11} - \epsilon^{*,\alpha}_{11}) + C^{\alpha}_{1122}(\bar{\epsilon}_{22} + \delta\epsilon^{\alpha}_{22} - \epsilon^{*,\alpha}_{22}) + 2C^{\alpha}_{1112}(\bar{\epsilon}_{12} + \delta\epsilon^{\alpha}_{12} - \epsilon^{*,\alpha}_{12}) \\ &= C^{\beta}_{1111}(\bar{\epsilon}_{11} + \delta\epsilon^{\beta}_{11} - \epsilon^{*,\beta}_{11}) + C^{\beta}_{1122}(\bar{\epsilon}_{22} + \delta\epsilon^{\beta}_{22} - \epsilon^{*,\beta}_{22}) + 2C^{\beta}_{1112}(\bar{\epsilon}_{12} + \delta\epsilon^{\beta}_{12} - \epsilon^{*,\beta}_{12}), \end{aligned} \tag{8}$$

$$\begin{aligned} &C^{\alpha}_{1112}(\bar{\epsilon}_{11} + \delta\epsilon^{\alpha}_{11} - \epsilon^{*,\alpha}_{11}) + C^{\alpha}_{2212}(\bar{\epsilon}_{22} + \delta\epsilon^{\alpha}_{22} - \epsilon^{*,\alpha}_{22}) + 2C^{\alpha}_{1212}(\bar{\epsilon}_{12} + \delta\epsilon^{\alpha}_{12} - \epsilon^{*,\alpha}_{12}) \\ &= C^{\beta}_{1112}(\bar{\epsilon}_{11} + \delta\epsilon^{\beta}_{11} - \epsilon^{*,\beta}_{11}) + C^{\beta}_{2212}(\bar{\epsilon}_{22} + \delta\epsilon^{\beta}_{22} - \epsilon^{*,\beta}_{22}) + 2C^{\beta}_{1212}(\bar{\epsilon}_{12} + \delta\epsilon^{\beta}_{12} - \epsilon^{*,\beta}_{12}). \end{aligned} \tag{9}$$

With the no-slip condition in this geometry, the displacements do no vary in the '2' direction. Therefore, $\delta\epsilon^{\alpha}_{22} = \frac{\partial u^{\alpha}_2}{\partial r_2} = 0 = \frac{\partial u^{\beta}_2}{\partial r_2} = \delta\epsilon^{\beta}_{22}$.

From (3), when the areas of α and β phase are equal,

$$\delta\epsilon^{\alpha}_{11} = -\delta\epsilon^{\beta}_{11}, \tag{10}$$

$$\delta\epsilon^{\alpha}_{12} = -\delta\epsilon^{\beta}_{12}. \tag{11}$$

From (8)–(11), we can solve for $\delta\epsilon^{\alpha}_{11}$ and $\delta\epsilon^{\alpha}_{12}$. From the global mechanical equilibrium condition, $\frac{\partial \sigma_{ij}}{\partial r_j} = 0$, all the strain components and thereby, the stress components, are constant within their respective phases. The non-zero heterogeneous strain and elastic stress components in the two phases are illustrated in Fig. 1(b).