



ELSEVIER

Contents lists available at SciVerse ScienceDirect

Journal of Crystal Growth

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

Implementation of an antitrapping current for a multicomponent multiphase-field ansatz

A. Carré, B. Böttger, M. Apel

ACCESS e.V., D-52072 Aachen, Germany



ARTICLE INFO

Article history:

Received 6 January 2013

Received in revised form

10 May 2013

Accepted 26 May 2013

Communicated by M. Plapp

Available online 31 May 2013

Keywords:

A1. Computer simulation

A1. Growth models

A1. Solidification

A1. Phase-field

B1. Alloys

ABSTRACT

The benefit of an antitrapping current has been investigated for a multicomponent multiphase-field model based on a double obstacle potential [Eiken et al., Phys. Rev. E 73 (2006) 066122]. Arguments justifying the analytical form of this correction for artificial solute trapping are given using Kim's formalism [Kim, Acta Mat. 55 (2007) 4391]. The validity of the model has been tested by comparing the phase-field results with those obtained by a sharp interface model. In particular, the 1D steady state solutions for solidification of a binary Al–Si and a ternary Al–Si–Mg alloy under isothermal conditions with a constant solute concentration at a finite distance from the solidification front have been used for comparison. The front velocity, the liquid concentration profile, and the concentration in solid predicted by the phase-field model with antitrapping compare well with the sharp interface solutions. In addition, for dendritic growth the convergence of tip velocity and local solute concentration at the tip with decreasing interface thickness is demonstrated.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

The key problem for the simulation of the microstructure evolution during phase transformation is a correct and effective description of the movement of the phase boundaries. In alloy solidification a moving phase boundary is in general associated with the redistribution of alloying elements. When assuming a sharp interface between the phases, the solute concentration profile is discontinuous over the interface and the concentration ratio for the local concentrations at both sides is given by the segregation coefficients. At low and moderate interface velocities the value of the segregation coefficient is given by the local thermodynamic equilibrium condition, for the absolute concentrations the interfacial curvature effect has to be considered. Thus, the solution of a sharp interface model requires an explicit tracking of the interface with local triangulation for curvature calculations. The phase-field approach avoids the issue of explicitly tracking the interface by introducing a diffuse interface description described by an order parameter which varies smoothly but steeply over the interface on the length scale η . Phase-field models can be derived from a sound thermodynamic basis which naturally leads to a diffuse interface on an atomistic scale [1].

In this paper we will follow the spirit of applied phase-field modelling when the diffuse interface is considered rather as a

convenient numerical vehicle to solve the free boundary problem than being a real physical property. In order to achieve accessible computation times, η is often selected as much larger than a physical interface width in the order of the finest microstructural details to be resolved in the simulation. However, the numerical solution should be independent of the choice of the interface thickness and must still reproduce the sharp interface results with a reasonable accuracy. A rigorous analysis of the sharp interface limit $\eta \rightarrow 0$ requires η to be much smaller than the capillarity length of the particular system. For a numerical solution of the phase-field equation this requirement on the spatial resolution can only be met for 1D problems or by extreme high performance computing [2]. The increase of the interface thickness η causes several artifacts leading to η depending phase-field simulation results. How severe this dependency shows up, depends on the particular simulation scenario, e.g. in the case of equiaxed solidification in casting the simulation of the initial growth, starting from nucleation until soft impingement is more prone to diffuse interface artifacts than the later stages. At higher solid fractions the diffusion fields become flat and the numerical requirements regarding η are less severe.

In order to relax the restrictions on the spatial resolution for quantitative phase-field simulations Karma and Rappel [3] introduced a thin interface analysis. In the first papers the thin interface asymptotic expansion has been developed for a thermal phase-field model with equal thermal conductivities on both sides (symmetric model) or no diffusion in the solid (one sided model). The thin interface limit leads to a correction of the interface

E-mail address: m.apel@access.rwth-aachen.de (M. Apel).

mobility based on an analysis of the temperature variation across the interface and thus corrects the local dependency of the driving force over the diffuse interface. Additional artifacts have been reviewed by Almgren [4]. For a solutal phase-field model the diffuse interface induces artificial solute trapping and modifies the mass conservation condition at the interface. Karma and Echebarria et al. [5,6] showed that these artifacts can be reduced by introducing an antitrapping term into the diffusion equation which compensates for the interfacial anomalies. A generalization of this latter approach has been proposed by Ohno and Matsuura [7,8] and by Pan and Zhu [9] in the case of an arbitrary solid diffusivity. More recently the phenomenological antitrapping model was also derived thermodynamically consistent for a variational phase field formulation [10] and also investigated in a more general context of basic principles of irreversible thermodynamics [11].

This work addresses the formulation of an antitrapping current suited for a multicomponent phase-field model based on a double obstacle potential [12]. A derivation of the antitrapping current will be given following the argumentation of Kim [13], the analytical results are consistent with the work of Choudhury and Nestler [14] based on a grand-potential formulation. However, unlike [14] the convergence of this ATC model to the sharp interface solution will be demonstrated by comparing it with the solutions of the sharp interface model. To that purpose the isothermal solidification of a binary AlSi alloy and the ternary case for an AlSi1Mg alloy including cross-diffusion effects has been considered.

The present paper is organized as follows. In Section 2 the double-obstacle phase-field ansatz for which we derived the antitrapping correction is presented, then in Section 3 analytical justifications are given for the antitrapping correction. Finally, comparisons of the model with one-dimensional numerical solutions of the sharp interface formulation and 2D simulations of dendritic growth are shown in Section 4.

2. Model

2.1. Free energy functional

From a numerical point of view, the phase-field approach replaces the explicit description of a sharp boundary which separates two adjacent phases or grains by a discontinuous jump of properties, e.g. from the solid to the liquid state, by a continuous order parameter function $\phi_\alpha(\vec{x}, t)$ whose scalar field gives the local phase or grain fraction at the position \vec{x} at the time t . $\phi_\alpha(\vec{x}, t)$ varies continuously over the interface, e.g. from 0 to 1, on a length scale η and the position of an equivalent sharp interface is defined by the $\phi(\vec{x}) = 0.5$ contour. Following the multiphase-field ansatz originating from [15], the phase-field parameter ϕ_α represents the local molar fraction of a phase α . For a dual interface between phases α and β $\phi_\alpha + \phi_\beta = 1$ holds. The local concentration of an element i , $c_i(\vec{x}, t)$, is given through the mixture rule [16]:

$$c_i(\vec{x}, t) = \sum_\alpha c_{i\alpha}(\vec{x}, t) \phi_\alpha(\vec{x}, t) \quad (1)$$

Using the above definitions one can express the free energy density f of the system by the sum over different contributions, namely: the interfacial contribution $f^{\text{intf}}(\{\phi_\alpha\})$, and the chemical free energy density $f^{\text{chem}}(\{\phi_\alpha\}, \{\vec{c}_\alpha\})$, $f = f^{\text{intf}} + f^{\text{chem}}$. The chemical free energy is assumed to follow also a mixture rule:

$$f^{\text{chem}}(\{\phi_\alpha\}, \{\vec{c}_\alpha\}) = \sum_\alpha h_p(\phi_\alpha) f_\alpha(\vec{c}_\alpha) \quad (2)$$

where f_α is the bulk free energy density of phase α , and $h_p(\phi)$ is a monotonic interpolation function fulfilling $h(0) = 0$ and $h(1) = 1$. In

the present model, \vec{c} denotes the n -tuple of concentrations of all n elements of the alloy, which can be reduced to $(n-1)$ by applying mass conservation.

The interfacial contribution to the free energy density is given by a combination of potential and gradient energy contributions as follows:

$$f^{\text{intf}} = \sum_{\alpha, \beta > \alpha}^\nu \left[W_{\alpha\beta} g_{\alpha\beta}(\phi_\alpha, \phi_\beta) - \frac{\epsilon_{\alpha\beta}^2}{2} \nabla_x \phi_\alpha \nabla_x \phi_\beta \right]. \quad (3)$$

In this paper, the function $g_{\alpha\beta}(\phi_\alpha, \phi_\beta) = \phi_\alpha \phi_\beta$ (for $0 \leq \phi \leq 1, \infty$ otherwise) is a symmetric function ("double obstacle") having a parabolic shape whose amplitude is scaled by $W_{\alpha\beta}$. The quantities $W_{\alpha\beta}$ and $\epsilon_{\alpha\beta}$ can be identified with the interfacial energy $\sigma_{\alpha\beta}$ by integrating both parts of Eq. (3) over the interface from $\phi = 0$ to $\phi = 1$. This leads to the relations $W_{\alpha\beta} = 4\sigma_{\alpha\beta}/\eta$ and $\epsilon_{\alpha\beta} = \sqrt{8\eta\sigma_{\alpha\beta}/\pi}$, see [12].

2.2. Multiphase-field model

The temporal evolution of the order parameter ϕ , i.e. the phase-field equation, is derived from a relaxation approach for non-conserved order parameters, based on the free energy $F = \int_\Omega f d\Omega$:

$$\frac{\partial \phi_\alpha}{\partial t} = - \sum_{\beta \neq \alpha}^\nu \mu_{\alpha\beta}^* \left(\frac{\delta F}{\delta \phi_\alpha} - \frac{\delta F}{\delta \phi_\beta} \right), \quad (4)$$

$\delta F/\delta \phi$ being the functional derivative of the free energy and $\mu_{\alpha\beta}^*$ the phase-field interface mobility. Using the analytical expression of Eqs. (2,3) for the energy densities, Eq. (4) can then be further expanded:

$$\frac{\partial \phi_\alpha}{\partial t} = \sum_{\beta \neq \alpha}^\nu \mu_{\alpha\beta}^* \left[h'_p \Delta G_{\alpha\beta} - \sigma_{\alpha\beta} K_{\alpha\beta} + \sum_{\gamma \neq \beta \neq \alpha} J_{\alpha\beta\gamma} \right] \quad (5)$$

where $\Delta G_{\alpha\beta}$ represents the thermodynamic driving force:

$$\Delta G_{\alpha\beta} = f_\beta(\vec{c}_\beta) - f_\alpha(\vec{c}_\alpha) - \sum_{i=1}^{n-1} \tilde{\mu}_i (c_{i\beta} - c_{i\alpha}) \quad (6)$$

weighted by h'_p . In the present formulation this weighting function has been defined $h_{p,\alpha\beta}' = \frac{\pi}{\eta} (\phi_\alpha + \phi_\beta) \sqrt{\phi_\alpha \phi_\beta}$ in order to concentrate the thermodynamic force to the center of the interface. The terms $\tilde{\mu}_i (c_{i\beta} - c_{i\alpha})$ are derived from a Lagrange term $\sum_{i=1}^{n-1} (c_i - \sum_{\alpha=1}^\nu c_{i\alpha}) \mu^i$ added to Eq. (2) to ensure the local mass balance. In the following analysis, the driving force is approximated by means of a linearized phase diagram centered at the melting temperature of the matrix component T_m :

$$\Delta G_{\alpha\beta} = \Delta S_{\alpha\beta} \left(T_m - T + \sum_i m_{i,\alpha\beta}^l c_{i\alpha} \right) \quad (7)$$

with the liquidus slope $m_{i,\alpha\beta}^l < 0$, $\Delta S_{\alpha\beta}$ is the entropy of transformation per volume. The pairwise curvature contributions to the interfacial curvature contribution are

$$K_{\alpha\beta} = \frac{\pi^2}{2\eta^2} (\phi_\beta - \phi_\alpha) + \frac{1}{2} (\nabla_x^2 \phi_\beta - \nabla_x^2 \phi_\alpha) \quad (8)$$

and the third-order junction forces

$$J_{\alpha\beta\gamma} = \frac{1}{2} (\sigma_{\beta\gamma} - \sigma_{\alpha\gamma}) \left(\frac{\pi^2 \phi_\gamma}{\eta^2} + \nabla_x^2 \phi_\gamma \right) \quad (9)$$

For a dual interface with $\phi_\beta = 1 - \phi_\alpha$ the phase-field equation in the present notation reads like

$$\frac{\partial \phi_\alpha}{\partial t} = \mu_{\alpha\beta}^* \left[\frac{\pi}{\eta} \sqrt{\phi_\alpha (1 - \phi_\alpha)} \Delta G_{\alpha\beta} - \sigma_{\alpha\beta} \left(\frac{\pi^2}{2\eta^2} (1 - 2\phi_\alpha) - \nabla_x^2 \phi_\alpha \right) \right] \quad (10)$$

Download English Version:

<https://daneshyari.com/en/article/8152218>

Download Persian Version:

<https://daneshyari.com/article/8152218>

[Daneshyari.com](https://daneshyari.com)