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From wetting to melting along grain boundaries using phase field and sharp interface methods

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ABSTRACT

We investigate the ability of a multi-order parameter phase field model with obstacle potentials to describe grain boundary premelting in equilibrium situations. In agreement with an energetic picture we find that the transition between dry and wet grain boundaries at the bulk melting point is given by the threshold $2\sigma_{sl} = \sigma_{gb}$, with σ_{sl} being the solid-melt interfacial energy and σ_{gb} the energy of a dry grain boundary. The predictions for premelting are confirmed by simulations using the phase field package OpenPhase. For the prediction of the kinetics of melting along grain boundaries in pure materials, taking into account the short ranged interactions which are responsible for the grain boundary premelting, a sharp interface theory is developed. It confirms that for overheated grain boundaries the melting velocity is reduced (increased) for non-wetting (wetting) grain boundaries. Numerical steady state predictions are in agreement with a fully analytical solution in a subset of the parameter space. Phase field simulations confirm the predictions of the sharp interface theory.

1. Introduction

Grain boundaries are naturally present in many materials, and their understanding is essential for improving their properties. In particular at higher temperatures grain boundary induced failure can occur, for example during hot cracking [1]. Here in particular grain boundary melting [2] can play a significant role, caused by the overlap of adjacent solid-melt interfaces, which lead to an effective interaction between them, expressed through the so called disjoining potential. This effect has been studied experimentally [3–5], theoretically [6,1], and computationally, using lattice models [7,8], molecular dynamics or Monte Carlo simulations [9,10], phase field models [11], orientational order parameter phase field models [12,13], phase field crystal [14–17] and amplitude equations descriptions [18–20]. For a recent broad overview on the formation of quasi-two-dimensional phases at grain boundaries, also known as complexions, we refer to [21]. In general, high angle grain boundaries tend to premelt, i.e. a thin melt layer can appear along the grain boundary already below the bulk melting point. This effect is most pronounced in alloys, where grain boundary disordering can start around 60–85% of the bulk solidus temperatures. In the case of tungsten based binary alloys this strongly affects the sintering behaviour [22], and generally the grain boundary diffusivity [23]. Energetically, the ratio of the dry grain boundary energy σ_{gb} to twice the value of the solid-melt interfacial energy $2\sigma_{sl}$ is the relevant parameter at the melting temperature T_M: For $\sigma_{gb}/2\sigma_{sl}$ larger (smaller) than one the dry grain boundary is energetically less (more) favourable; hence one expects a repulsive (attractive) interaction between the solid-melt interfaces.

In this article we investigate how grain boundary premelting appears in phase field models, which are frequently used for various aspects of microstructure evolution [24–28]. The multi-order parameter phase field model [29] is often used for the simulation of such problems. It is the basis of the phase field codes Micress [30] and OpenPhase [31]. In a phase-field context, interactions between solid-melt interfaces appear when the smooth order parameter profiles with a width ξ overlap. Despite the similarity to other models with a double well potential [32], the premelting behaviour is different here [11,33]. Next to a theoretical analysis we perform here numerical simulations to validate the predictions of the short ranged interactions and grain boundary premelting.

Beyond equilibrium situations the kinetics of grain boundary premelting is of highest interest. Recently, the heterogeneous nucleation of liquid droplets at overheated grain boundaries has been studied using atomistic and continuum methods [34]. This way, a framework has been developed to incorporate the aforementioned short ranged interactions to nucleation processes. The subsequent growth regime in the diffusion limited case has been

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studied in [35] using sharp interface methods. In contrast to [36] also the effect of the disjoining potential has been considered there. A central outcome is that it has – although relevant only in the triple junction region formed by the advancing melt front with the grain boundary – a quite substantial influence on the melting velocity. In the present article we aim additionally at a complementary modelling using phase field descriptions.

The article is organised as follows: In Section 2 we introduce the multi-order parameter phase field model, which is the basis for the theoretical and numerical investigations of grain boundary premelting and the wetting kinetics in this article. Section 3 is devoted to static equilibria. The analytical prediction of the premelting of planar grain boundaries is presented in Section 3.1. A complementary numerical investigation using the OpenPhase code is made in Section 3.2. The kinetics of the wetting of a low angle grain boundary is discussed in Section 4. The simulation of this phenomenon by phase field simulations in Section 4.1 is followed by a sharp interface analysis in Section 4.2, including a comparison of the two perspectives. The main results are summarised in Section 5.

2. The multi order parameter phase field model

Since the multi-order parameter phase field model by Steinbach and Pezzolla [29] plays a central role for the analysis and simulations in this article, we concisely summarise the governing equations here. In the basic situation of a single component, multiphase or polycrystalline structure the model is described by the free energy

$$F_0 = \int \left\{ \sum_{\alpha=1}^{N} \sum_{\beta>\alpha}^{N} \left(\frac{-4\eta_{\alpha\beta}\sigma_{\alpha\beta}}{\pi^2} \nabla\phi_\alpha \nabla\phi_\beta + \frac{4\sigma_{\alpha\beta}}{\eta_{\alpha\beta}} \phi_\alpha \phi_\beta \right) - \frac{L(T-T_M)}{T_M} [1 - g(\{\phi_\alpha\})] \right\} dV. \quad (1)$$

The dimensionless phase fields (order parameters) ϕ_α, which vary between 0 and 1, distinguish between the phases or grains. In the summations, N is the maximum number of phases which may appear in the description. The constraint

$$\sum_{\alpha}^{N} \phi_\alpha = 1, \quad (2)$$

which has to hold everywhere, allows to interpret the phase fields as local volume fractions of the phases. In contrast to models with a double- or multi-well potential, the confinement of the order parameters to the interval $\phi_\alpha \in [0:1]$ is enforced by an infinite energy penalty if the phase field values are outside this domain. This is formally described by an additional energy term

$$F = F_0 + \begin{cases} 0 & 0 \leqslant \phi_\alpha \leqslant 1, \alpha = 1, \ldots, N \\ \infty & \text{else.} \end{cases} \quad (3)$$

This so called multi-obstacle potential strictly confines the smoothing of the phase fields at an interface to a finite layer. The other parameters in Eq. (1) are the interfacial energies $\sigma_{\alpha\beta} = \sigma_{\beta\alpha}$ (dimension: energy/area) and the interface thicknesses $\eta_{\alpha\beta} = \eta_{\beta\alpha}$ (dimension: length). In the following we assume that one of the order parameters stands for a melt phase. The tilt function $g(\{\phi_i\})$, which we do not specify here yet, interpolates between the liquid and the solid; particular choices will be discussed later. Therefore, deviations of the temperature T from the melting temperature T_M favour energetically either the solid or liquid phase. This term also contains the latent heat L (dimension: energy/volume).

A specific feature of the model is that the evolution of the microstructure is expressed in terms of interface fields

$$\dot{\psi}_{\alpha\beta} := -\left(\frac{\delta}{\delta\phi_\alpha} - \frac{\delta}{\delta\phi_\beta} \right) F, \quad (4)$$

such that the phase field evolution in the interface regions, $0 < \phi_\alpha < 1$, reads

$$\dot{\phi}_\alpha = \frac{1}{\widetilde{N}} \sum_{\beta\neq\alpha} \mu_{\alpha\beta} \dot{\psi}_{\alpha\beta}, \quad (5)$$

with kinetics coefficients $\mu_{\alpha\beta} = \mu_{\beta\alpha} > 0$. Here, $\widetilde{N}$ is the number of phases with non-vanishing volume fractions at the present position. Since this number is different in situations with a binary interface, a triple junction or overlapping interfaces, it is obvious that also the interface profiles are determined in a piecewise manner. These regions have to be connected by appropriate boundary conditions, as discussed in detail in [33].

3. Grain boundary wetting

3.1. Analytical solution

As discussed in the introduction, the premelting at a grain boundary in a phase field model appears via the overlap of the interface profiles. Such a situation is shown in Fig. 1, where we use three order parameters to distinguish the phases and grains.

In particular, we use here ϕ_1 and ϕ_2 for the two distinct solid grains and ϕ_3 for the melt phase. Planar interfaces are assumed in Fig. 1, therefore the phase fields have a nontrivial dependence only in the interface normal direction (x direction) and are translational invariant in the others. Effectively, the problem therefore becomes one-dimensional. As discussed in [33] it is not sufficient to use a single order parameter phase field model, which only distinguishes between solid and melt, but not between the grains. In that case, there is no grain boundary energy associated with the interface between them, and the interaction of the two solid-melt interfaces is always attractive. This implies that grain boundary premelting does not occur in such a situation. In contrast, for the multi-order parameter case, the premelting transition is directly linked to the ratio of the grain boundary energy to the solid-melt interfacial energies and correctly captured by the phase field model [33].

In the following we briefly summarise the steps to solve this problem analytically for a specific choice of the thermal coupling function $g(\{\phi_\alpha\})$, which serves as a benchmark for the comparison with phase field simulations using OpenPhase in the following subsection. There, also other choices of the coupling function will be discussed. The particular case

$$g(\phi_1, \phi_2, \phi_3) = 1 - \phi_3 \quad (6)$$

has the advantage that the equilibrium phase field equations are linear, and therefore their solution is straightforward.

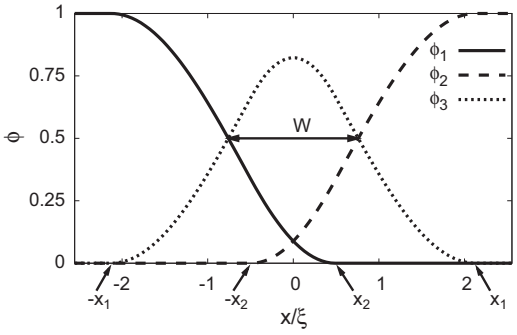

Fig. 1. Overlapping phase field profiles, as obtained from the analytical solution of the problem. Parameters are $\sigma_{gb}/\sigma_{sl} = 3$ and $\Delta_{13} = 0.25$. The melt layer thickness W is defined as the distance between the points where $\phi_3 = 1/2$.