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General evolution equation for the specific interface area of dendrites during alloy solidification



H. Neumann-Heyme ^a, K. Eckert ^{a,b}, C. Beckermann ^{c,*}

^a Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01314, Dresden, Germany

^b Institute of Process Engineering, Technische Universität Dresden, 01062, Dresden, Germany

^c Department of Mechanical and Industrial Engineering of Iowa, University of Iowa, Iowa City, IA, 52242, USA

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ABSTRACT

The specific area of the solid-liquid interface of an assembly of dendrites is an important integral measure of the morphology of the microstructure forming during alloy solidification. It represents the inverse of a characteristic length scale and is needed for the prediction of solidification defects and material properties. In the present study, the evolution of the interfacial area of dendrites is analysed using 3D phase-field simulations. A general evolution equation is developed for the specific interface area as a function of time and solid volume fraction that accounts for the effects of growth, curvature-driven coarsening and interface coalescence. The relation is validated using data from previously performed synchrotron X-ray tomography and isothermal coarsening experiments. It is found to be valid for arbitrary and even varying cooling rates and for a wide range of binary alloys. The rate constant in the evolution equation is successfully related to alloy properties.

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1. Introduction

Dendrites are the primary microstructure in virtually all metal alloys solidified from the melt. Their morphology is critical to the formation of solidification defects, such as porosity, cracks and macrosegregation. Dendrites also control the distribution of alloying elements on a microscopic scale and thereby the amount and spatial arrangement of secondary phases, which in turn strongly affect the properties of solidified materials. Understanding the evolution of dendrites during alloy solidification is thus of both fundamental and technological interest [1]. The most common measure for characterizing solidification microstructures and correlating material properties is the secondary dendrite arm spacing. Clearly, this spacing is an incomplete description of the complex shape of dendrites. As described in our earlier work on this topic [2], the specific area of the solid-liquid interface is an integral measure that characterizes the overall morphology in a more general sense [3,4]. The specific interface area S_s is defined as the area of the solid-liquid interface A per volume of the enclosed solid phase V_s ,

$$S_s = A/V_s \quad (1)$$

The inverse of the specific interface area can be considered a characteristic length scale of the microstructure. A similar integral measure is the interfacial area density or concentration S_V . It is defined as the interface area A divided by the sample volume V containing both solid and liquid phases,

$$S_V = A/V = g_s S_s \quad (2)$$

where $g_s = V_s/V$ is the solid volume fraction. The interfacial area density is a key ingredient in volume-averaged (macroscopic) models of alloy solidification [5]. It is needed, for example, in the modeling of microsegregation and of melt flow through the semi-solid mush, the permeability of which is directly related to S_V via the Kozeny-Carman relation $P \sim (1 - g_s)^3/S_V^2$ [6].

Under isothermal conditions, the interface area decreases continually due to surface energy driven coarsening, even though the amount of solid does not change. This temporal variation can be described by a classical coarsening law of the form [3]

$$S_s^{-1} = \left(S_{s0}^{-n} + Kt \right)^{1/n} \quad (3)$$

where S_{s0} , n , K , and t are specific interface area at $t = 0$, inverse

* Corresponding author.

E-mail address: becker@engineering.uiowa.edu (C. Beckermann).

coarsening exponent, coarsening rate constant, and time, respectively. An exponent of $n = 3$ has been firmly established for volume diffusion-limited coarsening by both experiments and theory. It was first obtained in the LSW theory for Ostwald ripening [7–9] that describes the evolution of a system of dispersed spherical particles in the long-time limit. Although the LSW theory assumes spherical particles and $g_s \rightarrow 0$, $n = 3$ has been found to be valid for more general geometries [3,10], including morphologies that are initially dendritic, and for higher solid volume fractions, e.g. Ref. [11]. The coarsening rate constant K is generally a function of the solid fraction. More recently, a LSW-type model has been derived for the important case of concurrent growth and coarsening [12]. Although this model is also limited to low g_s , $n = 3$ was obtained even in the presence of net solidification.

As opposed to pure coarsening, solidification implies that the system is not isothermal (i.e., the cooling rate \dot{T} is non-zero) and the solid fraction g_s increases with time. Initially, the growth of the solid leads to an increase in the interface area. However, at higher solid fractions the evolution of the solid morphology becomes strongly affected by solutal interactions and by interface coalescence, which causes the interface area to decrease. For pure growth processes, in the absence of coarsening, the interfacial area density S_V can be correlated to g_s by an equation of the form

$$S_V = c g_s^p (1 - g_s)^q \quad (4)$$

where c , p , and q are constants. According to Eq. (4), with increasing solid fraction S_V first experiences a rise due to the creation of interfacial area by growth, goes through a maximum, and then decreases due to impingement and coalescence of interfaces. Various values for the constants p and q have been suggested. Speich and Fisher [13] found that data from recrystallization experiments could be described by $p = q = 1$. A computational model for the growth and impingement of grains confirmed these exponents [14]. Other suggestions have been $p = q = 2/3$ [15] and $p = q = 1/2$ [16]. A more detailed geometrical model of growing and impinging spheres has revealed that the constants c , p , and q are influenced by the nucleation kinetics and the spatial arrangement of the spheres [17]. Therefore, it is not possible to identify generally valid values for the constants in Eq. (4).

In summary, the basic Eqs. (3) and (4) for the evolution of the interface area are limited to seemingly opposing cases. Eq. (3) is valid only for isothermal conditions ($\dot{T} = 0$, $g_s = \text{const.}$), where the interface area decreases with time due to coarsening. Eq. (4), on the other hand, describes processes where g_s increases due to growth ($\dot{T} \neq 0$), but the interface area does not change when $g_s = \text{const.}$ Hence, the question remains how the two evolution equations can be combined to cover the general case of simultaneous growth and coarsening. Due to the length scales involved with dendrites, both phenomena are important in most alloy solidification processes.

The direct study of the morphological evolution of dendritic microstructures during alloy solidification has become possible due to two relatively recent developments: (i) the availability of computational tools, in particular the phase-field method [18] and high performance parallel computing platforms, to allow three-dimensional simulations to be conducted for realistic material properties and relatively large length and time scales, and (ii) the use of enhanced synchrotron and X-ray facilities to perform tomography in real time during solidification with sufficient resolution to measure the geometry of dendrites. In the present study, phase-field simulations of dendritic solidification of a binary alloy are used to study the variation of the interfacial area with solid fraction and time. The simulations extend our previous results [2] for a single to multiple cooling rates, including an isothermal

coarsening case. A new specific interface area evolution equation is proposed that fits the simulation data over the entire range of cooling rates. Then, data from previously performed high-speed synchrotron X-ray tomography solidification [19–22] and isothermal coarsening [23–25] experiments involving different alloy systems are used to validate the general interface evolution equation.

2. Phase-field simulations

2.1. Computational model

The 3D phase-field model used in the present study is the same as in Ref. [2]. For completeness, it is briefly described in the following. We employ the well-established phase-field model for directional solidification of a dilute binary alloy of Echebarria et al. [26], which assumes that the dendrites grow in a constant temperature gradient G that moves at a constant velocity V_p . The model is extended to account for solute diffusion in the solid [27].

The material data used in all simulations of the present study are representative of an Al-Cu alloy. They are given by an initial alloy solute concentration $C_0 = 6$ wt.%, liquidus slope $m = -2.6$ K/wt.%, melting point of pure aluminum $T_m = 660$ °C, partition coefficient $k = 0.14$, solute mass diffusivities in the liquid $D_l = 3000$ $\mu\text{m}^2/\text{s}$ and solid $D_s = 0.3$ $\mu\text{m}^2/\text{s}$, respectively, Gibbs-Thomson coefficient $\Gamma = 0.24$ μmK , and surface energy anisotropy coefficient $\varepsilon_4 = 0.02$. As illustrated in Fig. 1a, the computational domain covers a 1/8 sector of a dendrite by using available symmetries. The simulation domain has a width of 70 μm , which represents one half of the primary dendrite spacing, and a length in the direction of the temperature gradient of 350 μm . The boundaries are characterized by no-flux conditions. A small paraboloid at the bottom of the domain is used as the initial geometry of the solid. When the dendrite tip impinges on the upper wall, the simulation proceeds and the previously grown structure continues to solidify (see Fig. 3 below). The initial temperature of the liquid is taken as the dendrite tip temperature during steady growth; the dendrite tip undercooling was determined iteratively from preliminary simulations.

The phase-field model was implemented numerically using the parallel FEM library AMDiS [28,29]. It allows for adaptive mesh refinement, an example of which is shown in Fig. 1b. For the base case simulation, the smallest element size was 0.153 μm , which can be compared to a steady state primary dendrite tip radius in the base case simulation of 2.7 μm . The problem size was on average

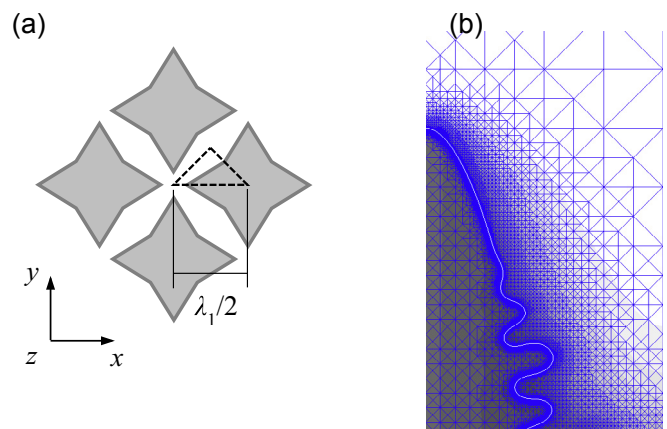


Fig. 1. Computational model: (a) assumed arrangement of the dendrites normal to the temperature gradient and triangular cross section of the calculation domain; (b) example of the adaptive mesh refinement used near the solid-liquid interface.

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