Dendritic and Eutectic Pattern Formations:

3D Phase-Field Simulations

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Abstract

Dendrites and eutectic growth structures are the most widely occuring pattern formations in metallic materials such as Fe-, Al- and Ni- based alloys. Nowadays, computer simulations provide the facility to enlight the growth process and to study the most important quantities influencing its quality. To model complex dendritic and eutectic solidification patterns, we formulated a non-isothermal phase-field model for multicomponent and multiphase systems in [1, 2]. The new model is capable to simultaneously describe the diffusion processes of multiple components, the phase transitions between multiple phases and the development of the temperature field. To numerically solve the set of governing equations we accomplish both, a parallel finite difference and an adaptive finite element method. Two- and three-dimensional simulations of dendritic array formation and of oscillatory binary eutectic microstructures are presented.

1 Introduction

Materials science plays a tremendous role in modern engineering and technology since it is the basis of the entire microelectronics and foundry industry, as well as many other industries. The manufacture of almost every man-made object and material involves phase transformations and solidification at some stage. Metallic alloys are the most widely-used group of materials in industrial applications. In metals, the most important phase transformations are of dendritic and eutectic type. Depending on the process conditions and on the material parameters, different growth morphologies and microstructure characteristics such as typical spacings between dendrites or between eutectic lamellae can be observed. The solidification process involves the formation of polycrystalline grain structures, dendritic arrays and interdendritic eutectics at different length and time scales which influence each other. Examples of experimental photographs are given in Fig. 1. The first image (Fig. 1 a)) shows the grain configuration of a polycrystalline Al-Si structure after a special preparation procedure of electrolytical etching. This grain structure contains grain boundary triple junctions which themselves have their own physical behaviour and obey their own physical laws. The coarsening by motion of the grain boundaries takes place on a long time scale.

If the magnification of the microscope is enlarged, a dendritic substructure of the crystals can be resolved (Fig. 1 b)). Each orientational variant of the grain structure consists of a dendritic array in which all dendrites that belong to a specific grain have the same crystallographic orientation. The third image in Fig. 1 c) visualizes the interdendritic eutectic structure on a microscopic scale where eutectic lamellae solidify between the primary dendritic phase. In such a eutectic solidification, two distinct solid phases S_1 and S_2 grow into an undercooled melt if the temperature is below the critical eutectic temperature. Within the interdendritic eutectic lamellae, a phase boundary triple junction of the two solid phases and the liquid phase can be considered. The dendrites and the eutectic lamellae grow into the melt on a microscopic scale during a short period of time. Once the dendrites and the eutectic lamellae impinge one another, grain boundaries are formed on a mesoscopic length scale.

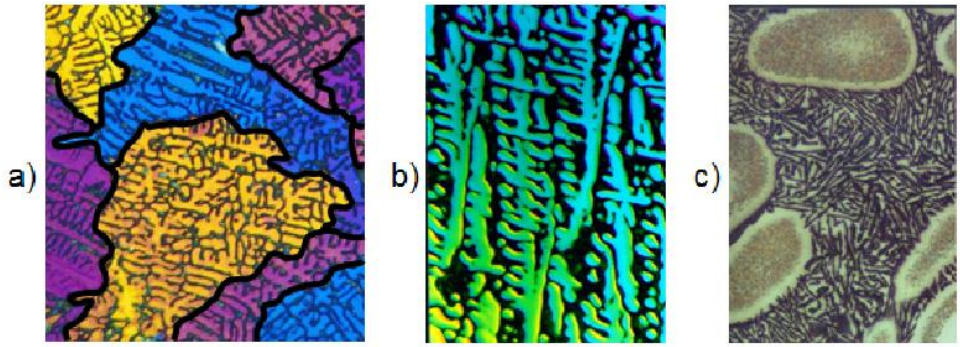

Figure 1: Experimental photographs of an $Al - Si$ alloy sample: a) Grain structure, b) network of primary Al dendrites and c) eutectic microstructure of two distinguished solid phases in the regions between the primary phase dendrites.

Mathematical modeling of physical and technological processes in materials science is the key to understanding and controlling the processes and to sustaining continuous progress in the field of optimizing and developing materials.

2 Phase-field Modeling

Traditionally, phase transitions have been described mathematically by moving free boundary problems in which the interface is represented by an evolving surface of zero thickness on which boundary conditions are imposed to describe the physical mechanisms occuring there. For an overview we refer to the recent book of Visintin [3]). Across the sharp interface certain quantities (e.g., the heat flux, the concentration or the energy) may suffer jump discontinuities. In practical computations, the sharp interface formulation leads to difficulties when the interface develops a complicated geometry or when topology changes occur. In recent years, the phase-field method has become an important tool for tackling

free boundary problems such as grain boundary motion and for simulating crystal growth, solidification and pattern formation phenomena in alloys. The advantage of the phase-field method lies in the formulation of diffuse interfaces of a finite thickness. Explicit front tracking is avoided by using smooth continuous variables locating the grain and phase boundaries. This alternative modeling technique requires much less restrictions on the complexity of the topology of the grain and phase boundaries. In the light of this, the particular strength of the diffuse formulation lies in its simple computational applicability to simulate the temporal evolution of complex interfacial shapes associated with realistic features of solidification of alloys.

The phase-field methodology is based on the construction of a Cahn-Hilliard or Ginzburg-Landau free energy functional. To formulate a phase-field model, an order parameter $\phi(\vec{x}, t)$, called the phase-field variable is introduced whose value characterizes the phase state of the system in time and space. In a standard phase-field approach for solid-liquid systems, $\phi(\vec{x}, t) = 1$ represents the solid and $\phi(\vec{x}, t) = 0$ the liquid phase. In contrast to classical sharp interface models, the interfaces are represented by thin diffuse regions in which $\phi(\vec{x}, t)$ varies between the values of ϕ associated with the adjoining bulk phases, i.e. $0 < \phi(\vec{x}, t) < 1$ as shown in Fig. 2. The diffuse interface profile is schematically drawn in Fig. 3.

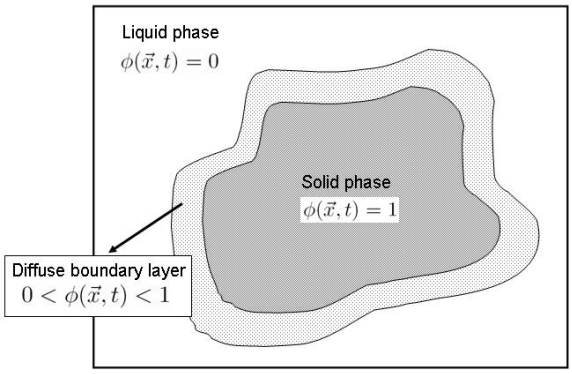

Figure 2: Schematic drawing of a solid particle surrounded by a liquid phase with a mushy zone in the region of the diffuse interface of the phase-field model.

The mathematical model comprises partial differential equations for the appropriate thermodynamic quantities (e.g. the concentration fields of the multiple components or the temperature) with an additional reaction-diffusion equation for the phase field, often called the phase-field equation. The equations contain a number of physical parameters of the real material such as the latent heats, the melting temperatures, the diffusion coefficients for each alloy component, the heat diffusion coefficient, the heat capacity, the surface energies, the kinetic coefficients and anisotropy data. The full set of equations is derived from an entropy functional in a thermodynamically consistent way in [1]. Examples of the energy contributions and the relation to the physical data are given in [2].

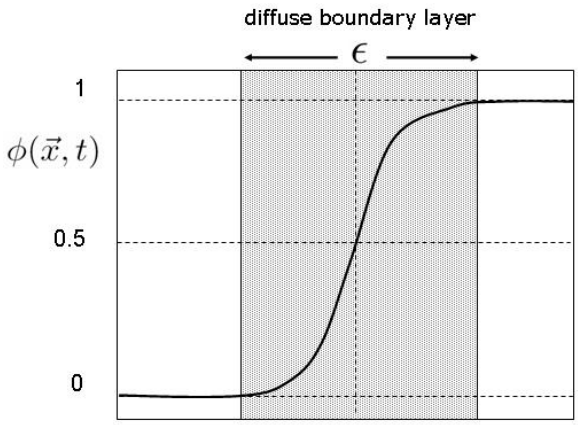

Figure 3: Diffuse interface profile of the phase-field variable varying smoothly from zero to one.

3 Application to dendritic and eutectic solidification

The computational applicability of phase-field models to alloy systems in three dimensional domains is restricted mostly due to the limited computer resources with respect to memory and CPU power. In numerically solving phase-field equations, the complexity of the up to date models require the development of highly efficient implementation algorithms. We have implemented two numerical methods based on (i) parallel finite differences, [4] and (ii) adaptive finite elements, [5]. For computations, it is required that the spatial resolution of the numerical method must be greater than the thickness of the diffusive phase boundary layer. The interfacial thickness itself must be less than the characteristic scale of the growing microstructure. In this case, a non-uniform grid with adaptive refinement as shown in Fig. 3 can dramatically reduce the use of computational resources against a uniform grid with the same spatial resolution.

The two- and three-dimensional simulations of dendritic growth in Fig. 5 were performed using the physical data of pure Nickel, [6]. A small amplitude of Gaussian distributed noise was added to the front, strong enough for dendritic side branches to evolve. The solidification of Ni starting from a rough front leads to several initial dendrite tips. A quick selection of the tip spacing due to the retarding effect of the emitted latent heat at the front follows, so that only a few dendritic fingers survive. The array of dendrites emerge with a 15° inclined orientation with respect to the surface normal. Due to the compact growth pattern, only minor side arm formation appears.
To simulate binary eutectic phase transitions, where two solid phases α and β grow into an undercooled melt, we have used the free energies belonging to a typical eutectic phase diagram as input data. For the computations in Fig. 6, we have considered an off-eutectic

composition of an $Al - Cu$ melt and observe a regular oscillatory growth mode of the two solids. The oscillations along the solid-solid interface are driven by the motion of the triple junctions. A characteristic amlitude and wave length is established during the solidification. The 3D microstructure performs an alternating topological change from α-solid rods embedded in a β-matrix to β-solid rods embedded in an α-matrix and so on, Fig. 6 b).

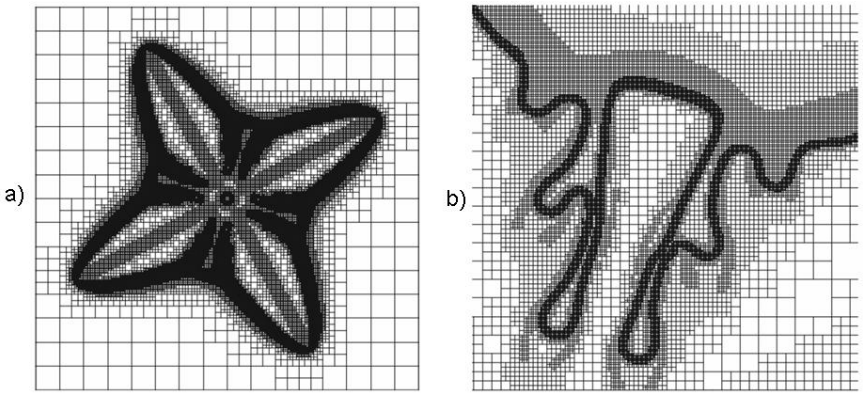

Figure 4: a) Adaptive grid of a finite element simulation of dendritic growth, b) interface region at higher resolution.

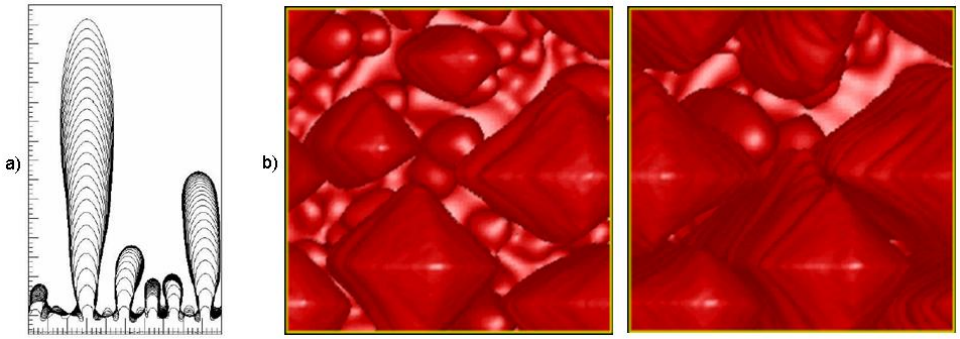

Figure 5: Phase-field simulations a) of two-dimensional dendritic growth in an undercooled pure Ni melt and b) of a three-dimensional selection process in a dendritic array with a 15° inclined orientation with respect to the surface normal.

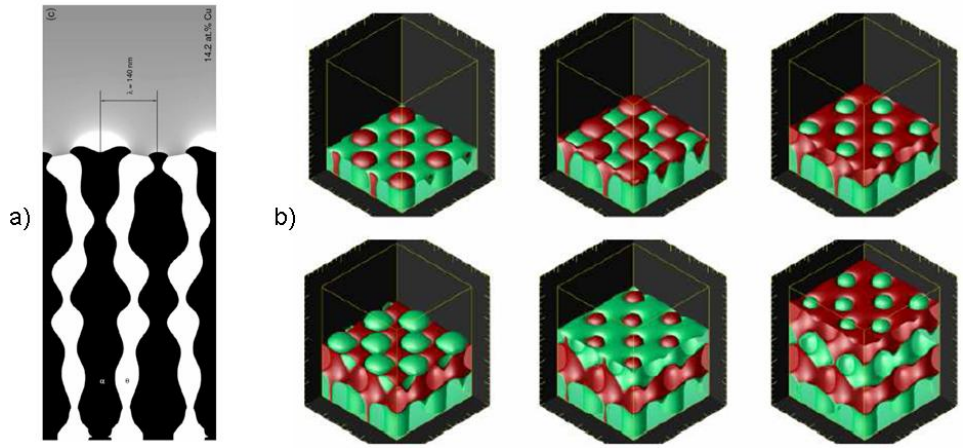

Figure 6: a) Regular oscillations along the solid-solid interface of a binary eutectic growth structure driven by the motion of the triple junction/triple line in 2D, b) topological change of the microstructure in 3D.

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