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Simulation of solid deformation during solidification: Compression of a single dendrite

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Abstract

A method is developed to numerically simulate coupled solidification and deformation of dendrites. Dendritic solidification is modeled using the phase-field method. The elasto-viscoplastic deformation of the growing solid is computed using the material point method. The stress analysis assumes a sharp and stress free solid–liquid interface, with the zero contour line of the phase field used to identify the interface. The deformation-induced flow in the liquid is approximated through a zero-gradient extension of the deformation velocities in the solid. Changes in the crystallographic orientation angle and advection of the phase and temperature fields due to solid deformation are all accounted for. Numerous tests are performed to validate the various numerical procedures. The full model is then applied to simulate in two dimensions the compression of a single dendrite of a pure substance growing in an undercooled melt. The development of complex stress and strain distributions is observed. The deformations result in variations in the crystallographic orientation angle within the dendrite that, in turn, affect the subsequent solidification behavior. The modeling of the deformation of polycrystalline solidifying structures, including the formation of grain boundaries, is described in a companion paper.

Keywords: Dendritic growth; Viscoplastic deformation; Phase-field method; Material point method

1. Introduction

Deformation of the solid is a common occurrence during metal casting processes [1,2]. Often the solid deforms simply due to thermal stresses, but sometimes the deformation is caused by external forces, for example through the rolls in continuous casting, mold wall movement, or an applied pressure. When the casting is still solidifying, the deformations can extend into the semi-solid mushy zone. This mushy zone is typically composed of solid dendrites surrounded by liquid. Deformation of the mush can lead to numerous defects in a solidified casting, including hot tears, macrosegregation and porosity. Therefore, understanding the mechanical behavior of mush is of great interest for advancing casting simulations incorporating a stress analysis and, ultimately, for preventing defects in castings [3].

The overall goal of the present study is to develop a numerical method for simulating the deformation of a solidifying mush on the scale of the evolving microstructure. Such direct numerical simulations may lead to improved constitutive models for use in macroscopic stress simulations. Mush deformation is a complex process involving multiple physical phenomena: solidification and formation of bridges or grain boundaries between dendrites, large inelastic solid deformation with contacts, liquid flow, etc. Simulating all of these processes simultaneously would be a very challenging task. A few researchers have developed methods to investigate the mechanical behavior of mush. Phillion et al. [4] and Fuloria and Lee [5] calculated inelastic deformation of multi-grain and dendritic microstructures, respectively, without considering solidification. Uehara et al. [6] performed thermal stress simulations in a confined solidifying microstructure. Fully

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coupled solidification and deformation simulations of dendritic microstructures have not been performed in the past. The coupling of the solidification and deformation calculations is important not only because the deformations are a function of the morphology of the evolving solid, but also because the solidification patterns are affected by the deformations. In order to simplify the problem, we focus in the present study on dendritic solidification and solid deformation of a pure substance in two dimensions. Stresses that are exerted by the liquid on the solid are neglected. This assumption is realistic when the liquid can "drain" freely. In fact, the flow of the liquid is not modeled at all. Transformation stresses/strains, stress-induced phase transformations, and heat generation due to inelastic deformation are not considered. These assumptions are all appropriate for a slowly deforming mush. All material properties are assumed to be constant, and the thermophysical properties of the solid and liquid are assumed to be equal.

The simulation of dendritic solidification with large solid deformations necessitates numerous choices regarding the models to be used and the numerical methods to be employed. The phase-field method [7,8] is used in the present study to simulate solidification. Since it employs a diffuse interface concept, it is especially well suited for handling morphological changes and singularities, such as those caused by portions of a dendrite impinging on one another. Such wetting and bridging phenomena are not well handled by traditional sharp interface approaches. In addition, phase-field methods are available to simulate solidification of multiple crystals while accounting for their individual crystallographic orientations and the formation of grain boundaries [9]. The main new feature of the present phase-field calculations is that due to the deformation of the solid, the crystallographic orientation angle is no longer uniform within a single dendrite and continuously evolves. Furthermore, the phase-field and the temperature field are advected by the deformation velocity. The stress model for simulating the elasto-viscoplastic deformation of the solid assumes that the solid–liquid interface is sharp. The zero contour line of the phase field is used to identify the interface. The stress model is only solved in the solid and the solid–liquid interface is taken as stress free. The numerical method employed in the solution of the stress model needs to be able to handle large strains, self-contact and impingement of solid. Particle methods or meshless methods are attractive for this purpose, because they do not suffer from the mesh collapse or entanglement problems typical of Lagrangian finite-element methods (FEMs). In the present study, the material point method [10] is selected. The main feature of this method is that is uses, as in a particle method, a Lagrangian description for the motion of material points, and a fixed Eulerian background mesh for solving the equation of motion. The latter feature makes the material point method well suited for coupling with the (Eulerian) phase-field method.

The present paper is limited to the simulation of the coupled solidification and deformation of a single dendrite. This simplification is made in order to allow for detailed testing and validation of the methods employed. Several examples are presented that illustrate the complex physical phenomena involved. A companion paper [11] then extends the present method to consider multiple dendrites and grain boundaries.

2. Models and numerical procedures

2.1. Phase-field method for dendritic solidification in the presence of solid deformation

The standard phase-field model of Karma and Rappel [12] is used to simulate dendritic solidification of a pure substance from an undercooled liquid melt. Let ϕ denote the phase field, where $\phi = \pm 1$ refers to the bulk solid and liquid phases, respectively. The anisotropic form of the two-dimensional phase-field evolution equation is given by:

$$\tau_\phi(\alpha)\left(\frac{\partial\phi}{\partial t} + \boldsymbol{v}\cdot\nabla\phi\right) = \nabla\cdot\left[W^2(\alpha)\nabla\phi\right] - \frac{\partial f(\phi,\lambda\theta)}{\partial\phi} + \frac{\partial}{\partial x}\left[|\nabla\phi|^2 W(\alpha)\frac{\partial W(\alpha)}{\partial\phi_x}\right] + \frac{\partial}{\partial y}\left[|\nabla\phi|^2 W(\alpha)\frac{\partial W(\alpha)}{\partial\phi_y}\right], \quad (1)$$

where $\tau_\phi(\alpha) = \tau_0\xi^2(\alpha)$ and $W(\alpha) = {}_0\xi(\alpha)$ are orientation-dependent relaxation time and diffuse interface thickness parameters, respectively, in which α is the (crystallographic orientation) angle between the interface normal and the crystal axes. The usual 4-fold crystalline anisotropy function $\xi = 1 + \varepsilon\cos(4\alpha)$ is used, where ε is the anisotropy strength of the surface energy. The phenomenological bulk free energy function is given by $f(\phi,\lambda\theta) = q(\phi) + \lambda\theta p(\phi)$, in which $q(\phi) = -\phi^2/2 + \phi^4/4$ is a double-well function and $p(\phi) = \phi - 2\phi^3/3 + \phi^5/5$ is an odd function. The dimensionless temperature is given by $\theta = (T - T_m)/(L/c_p)$, in which T, T_m, L and c_p are the temperature, melting point, latent heat and specific heat, respectively. The coupling constant, λ, and the relaxation time, τ_0, are chosen in accordance with the thin-interface analysis of Karma and Rappel [12] in order to model kinetics-free growth. The parameter W_0 has to be reduced until a converged solution that is independent of the diffuse interface thickness is obtained. The temperature field is obtained from the following heat equation:

$$\frac{\partial\theta}{\partial t} + \boldsymbol{v}\cdot\nabla\theta = D\nabla^2\theta + \frac{1}{2}\left(\frac{\partial\phi}{\partial t} + \boldsymbol{v}\cdot\nabla\phi\right), \quad (2)$$

where D is the thermal diffusivity. All other details can be found in the original Ref. [12].

The terms in Eqs. (1) and (2) involving the velocity vector, $\boldsymbol{v}$, account for advection of the phase field and the temperature field. Since Eqs. (1) and (2) are solved over the entire computational domain, the velocity field must be known everywhere. The deformation velocity in the solid

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