Available online at www.sciencedirect.com
ScienceDirect
Journal of Computational Physics 226 (2007) 131–155
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Modeling the growth and interaction of multiple dendrites in solidification using a level set method

Lijian Tan, Nicholas Zabaras *

Materials Process Design and Control Laboratory, Sibley School of Mechanical and Aerospace Engineering, 188 Frank H.T. Rhodes Hall, Cornell University, Ithaca, NY 14853-3801, USA

Received 15 December 2006; received in revised form 22 March 2007; accepted 29 March 2007
Available online 5 April 2007

Abstract

A level set method is presented to study the growth and interaction of multiple dendrites in solidification. The method couples thermal and solute diffusion with propagation of multiple interfaces. A single signed distance function is used to track the solid–liquid interface with the aid of markers, the value of which is the orientation angle, for identification of different crystals. The problem of evolving multiple crystal interfaces is reduced to two tasks: (1) tracking one level set variable (signed distance function) and (2) determination of the marker for a newly solidified finite element nodal point. Tracking a single level set variable is implemented by solving the level set equation with interface velocity computed from an extended Stefan equation using the marker information (crystal orientation). Determination of the marker for a newly solidified finite element nodal point is implemented by using an algorithm modified from the fast marching technique. Both of these two steps are computationally efficient and the approach is suitable for incorporating effects of multiple crystals. Convergence and accuracy of this approach are demonstrated by using different grid spacings and comparing with results obtained from the multi-phase level set method. A parametric study is performed to investigate the effects of solidification speed and thermal gradient on the resulting solidification microstructure pattern. Numerical results of columnar-to-equiaxed transition (CET) qualitatively agree with an analytical estimation and are similar to previous numerical results obtained using a phase field method. A convergence study is performed to determine the appropriate grid spacing for numerical simulation. At lower surface tension, CET occurs at a lower thermal gradient for a giving solidification speed. Secondary dendrite formation is more apparent with lower surface tension. The differences and similarities between the three-dimensional and two-dimensional growth results are analyzed. Randomness in crystal orientation and required undercooling for nucleation are modeled and found to have a great effect on the microstructure pattern. The efficiency of the present approach is finally demonstrated with an example that includes the growth of hundreds of crystals with consideration of randomness effects.

Keywords: Level set method; Multi-phase motion; Dendritic solidification; Crystal growth; Columnar-to-equiaxed transition

* Corresponding author. Tel.: +1 607 255 9104; fax: +1 607 255 1222.
E-mail address: zabaras@cornell.edu (N. Zabaras).
URL: http://mpdc.mae.cornell.edu (N. Zabaras).

0021-9991/$ - see front matter © 2007 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2007.03.023

1. Introduction

The formation of complex microstructure during solidification of pure materials and alloys has been of great interest for hundreds of years. Various numerical methods including cellular automata [1–4], front-tracking methods [5–8], phase field techniques [9–18] and level set methods [19–24] have been developed to study the growth of crystals and dendrites. Among these methods, the cellular automata technique is suitable for studying the interaction between multiple dendrites especially in three-dimensions (3D), because its computational requirement (memory and time) is low in comparison to other numerical methods. Cellular automata is widely used in many areas including biological systems and highway traffic modeling. In this technique, a collection of 'colored' cells on a grid of specified shape evolves through a number of discrete time steps according to a set of rules based on the states of neighboring cells. Cellular automata was first introduced into solidification systems in [25] with a growth kinetics model, which can reflect the growth along preferred directions (e.g. $\langle 1\,0\,0\rangle$ crystallographic orientations) during dendrite development. The basic idea of cellular automata for solidification is to mimic interface propagation by capturing nearby liquid cells to the solid body according to a certain criterion. In recent advances of this method, cellular automata is coupled with finite differences (CA-FD) [2,4] or the finite element (CA-FE) [1] by using a criterion based on numerical solution of temperature or solute concentration from finite differences or the finite element method. Curvature effects can also be taken into account [2]. Cellular automata for solidification is relatively easier to implement and requires less computational resources than most other numerical methods, including front-tracking, phase field method, and level set method. However, it has some deficiencies in its accuracy due to its discrete nature. For example, it is pointed out in [1] that cellular automata methods have a tendency to bias the results by introducing an anisotropy associated with the network of cells or sites. Although corrections can be introduced [1] to circumvent this problem, independence of the cellular automata results on the numerical grid size and mesh orientation is rarely demonstrated. It is also pointed out in [26] that cellular automata lacks the ability to accurately take into account the surface tension anisotropy effect, which is of great importance in dendritic growth.

Although cellular automata is very successful in predicting grain structures which account for interaction between many dendrites, many researchers are working on other more complicated and computationally more expensive methods since issues of accuracy are not sufficiently addressed by the cellular automata method. In fact, obtaining a converged solution for a single crystal independent of mesh orientation itself is a nontrivial task due to the existence of a moving interface during the solidification process [7,8,18,20–22]. During the last two decades, significant progress has been made in the simulation of single crystal growth using phase field methods [12,13,18]. These approaches, by considering a diffuse interface and a fixed-grid, avoid the need for applying temperature boundary conditions on the moving interface. A review of recent progress in phase field methods as applied to solidification processes is given in [18]. The basic idea of the phase-field method is to employ a phase-field variable Φ that varies smoothly from zero to unity between the two phases over the diffuse interface region, which has a small but numerically resolvable thickness. The phase field variable serves to distribute the interfacial forces over the diffused freezing region. It is governed by a phase-field control equation derived from the thermodynamics of phase transition [18]. Important physical mechanisms, such as curvature, anisotropy and kinetics effects, are implicitly incorporated in the phase-field control equation. This leads to many computational advantages. For example, one does not need to compute interfacial geometric quantities such as interface curvature and outward normal vector. But on the other hand, this also leads to a drawback of the phase field methods since there are a large number of parameters involved in the solution of the evolution equations to be determined. Some of these parameters are difficult to determine for accurate physical crystal growth simulation of real world materials. The front-tracking method, however, can avoid the difficulty of determining parameters, since a sharp interface model is directly solved. Recently front-tracking techniques have been used successfully to reproduce the complex dendritic structure in crystal growth in undercooled melts including effects such as liquid trapping, tip-splitting, side branching and coarsening [5,6,27]. Successful 3D front-tracking implementations including the effects of melt flow have been presented [8]. The advantages of front-tracking methodologies lie in their ability to directly enforce the freezing interface temperature (Gibbs–Thomson) relation and energy balance (Stefan condition). Unfortunately, many of the current implementations of these conditions do not allow global energy conservation even though they may satisfy the Stefan condition pointwise.