RULE-BASED LATTICE COMPUTER MODELS FOR SIMULATING DENDRITIC GROWTH

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Introduction

Dendritic crystal growth is commonly observed in metals and other materials that solidify with low entropies of fusion. A dendrite is a branched single crystal structure which freezes such that the branches (dendrite arms) grow in specific crystallographic directions. As the tip of each branch advances it is possible, depending on the local conditions, for oscillatory formation of additional arms to occur at locations just behind the tip.

The evolution of a dendrite depends on the complex interaction of several physical phenomena including latent heat evolution and its removal from the solid-liquid interface, solid-liquid interfacial energy, the influence of solid-liquid interface curvature on the equilibrium freezing temperature and the atomic mechanism of the crystal growth process. In alloys freezing over a temperature range the complexity is increased due to the influence of solute redistribution during freezing on the local liquidus temperature.

Dendritic growth is of major importance in metallic materials and particularly in the case of alloys of off-eutectic composition. Dendrite fragmentation, dendrite arm spacing, dendrite morphology and interdendritic fluid flow are factors that influence the final grain structure, microstructure, formation of porosity and hot tears, solute segregation and mechanical properties in as-solidified alloys.

Dendrites are termed as being either constrained or free. Constrained dendrites grow from a surface, in a columnar fashion, such that the growth direction of the primary dendrite arms is opposite to the direction of heat flow. Each dendrite usually contains many primary arms. On the other hand, free dendritic growth corresponds to the formation of individual dendrites which are in suspension in supercooled liquid. As the latent heat of fusion flows from a dendrite into this supercooled liquid, the dendrite grows radially producing an equiaxed shaped grain until it impinges on other growing dendrites. It is inappropriate to refer to a primary arm spacing in equiaxed dendritic structures. Constrained dendrites are only found in alloys (or other materials freezing over a temperature range) when growth takes place into a positive temperature gradient. Free dendritic growth can occur in pure metals (or other pure materials) and alloys.

In phases solidifying with cubic crystal structures, the dendrite arms are usually parallel to [100] directions. Secondary dendrite arms are therefore orthogonal to the primary arms and, likewise, the tertiary arms are orthogonal to the secondaries.

Theoretical Models of Dendritic Growth

Early theoretical models (1,2) considered the steady state growth of an isolated, branchless and isothermal or isoconcentrate needle dendrite in a one-component system. It was assumed that the dendrite shape conformed to a parabola of revolution and that growth was taking place into a supercooled pure melt. Therefore, the only transfer process that had to be taken into consideration was heat flow. Later theories attempted to take into account the time dependent features of dendrites viz. sidebranch formation behind the advancing tip. Experimental investigation of free dendritic growth in pure melts to assess these theories is extremely difficult. Some of the most informative data has been obtained from studies of the freezing of succinonitrile by Glicksman et al (3). Huang and Glicksman (4) have written an excellent overview of free dendritic growth in pure materials which includes an examination of the theories of tip growth and sidebranch formation for free dendritic growth as well as a discussion of these theories based on experimental studies on succioninitrile.

More recently a number of models have been proposed to explain the solidification of cellular/dendritic structures in a positive temperature gradient (5-10). The objectives of these models have been to predict the influences of alloy composition, temperature gradient and growth rate on the temperature, radius of curvature and liquid composition at the cell/dendrite tip and, also, on the primary arm spacing of the array. These models have been critically examined and compared with experimental data by Tewari and Laxmanan (11). Since the latent heat is removed from the advancing primary tips by conduction through the solid, in these models the only transport process to be considered in the liquid ahead of the tips is that of the solute.

Numerical Models of Dendritic Growth

To date, reported numerical computer models of dendritic growth have been confined to the growth of a free dendrite in a supercooled one-component pure melt (12-14). The heat transfer problem and the dendrite morphology are controlled by two conditions. The first is that the equilibrium freezing temperature at any point on the solid-liquid interface, T_E, is determined by the local interface curvature. This is known as the Gibbs-Thomson effect and the depression of the freezing temperature due to capillarity (assuming that the solid-liquid interface is convex towards the liquid) is given by,

$$\Delta T = \frac{\sigma T_m}{\Delta H . \rho}\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$$

(1)

where T_m is the equilibrium freezing temperature of a planar interface, σ is the solid-liquid interfacial energy, R_1 and R_2 are the radii of curvature of the surface in two directions at right angles, ΔH is the enthalpy of fusion and ρ is the density of the solid.

The second condition is that the latent heat released on freezing must be removed from the solid-liquid interface by conduction. Any heat transfer due to convection is not presently taken into consideration.

However, these models are unable to simulate the oscillatory formation and growth of dendrite arm branches behind the advancing tip. Hunt (14) comments that it is probable that the velocity of the dendrite tip oscillates very slightly and this leads to the branching.

Rule-Based Lattice Computer Simulation of Dendrite Growth

In the last decade a number of papers have been published relating to the use of 2D rule-based lattice models (cellular automata) for simulating solidification (15-18). Cellular automata are mathematical models that can be applied to systems where a number of factors interact to cause a complicated pattern of behaviour. The evolution of a dendritic crystal falls into this category, the macroscopic pattern of growth being determined, e.g. in the case of alloy dendrites, by solute redistribution on freezing, latent heat evolution and its removal from the freezing interface and the Gibbs-Thomson effect. A cellular automaton consists of a regular lattice of sites (cells) where each site may be described by one or more variables. The values of these variables at a particular site are updated in discrete time steps according to rules that take into account the values of surrounding sites.

The simplest model for simulating solidification assumes that each site on the lattice (which represents an amount of material) can have two values e.g. 0 and 1, where 0 represents a liquid site and 1 a solid site. At each time step all sites are tested to ascertain if they are liquid or solid. If a site is liquid, a rule will be applied governed by the states of the adjacent neighbours to determine if the site should solidify. In pure materials the dendritic mode of freezing is a consequence of restricted growth caused by two factors viz. latent heat evolution and capillarity. In alloys, there is also the additional factor of solute redistribution. To obtain a simulation of the solidification of a branched dendrite therefore requires such a growth restriction to be inbuilt. A very elementary cellular automaton model of a dendrite employing a cubic lattice assumed the growth restricting rule that a liquid site will change to a solid site only if one of its four nearest neighbours is in state 1 (19). Solidification in the model was initiated from a square shaped four cell seed.

Packard (15) developed a more sophisticated cellular automaton model for solidification to examine the influence of modelled parameters on macroscopic growth forms. As well as the discrete solidification condition referred to in the previous paragraph, he included a continuous variable at each site to simulate heat transfer. He also incorporated a solidification rule that took into account local surface curvature and a rule for accounting for latent heat evolution. He observed that the growth forms of modelled crystals depended on the magnitude of the Gibbs-Thomson effect. As the degree of influence of curvature on the freezing temperature was reduced the growth forms changed from amorphous to tendril like (characterised by tip splitting) to dendritic like structures exhibiting side branching.

From the observations referred to in the above paragraphs and the present investigations it is evident that modelled dendrite-like growth forms depend on the seed shape, lattice geometry, the rule governing solidification and the rules controlling the growth restricting factors. In comparison with actual dendrites the shapes can vary from extremely simplistic to highly realistic.

The purpose of the present study, which is ongoing, was to further examine the application of rule-based lattice modelling techniques to the simulation and understanding of branched dendritic growth.

The Present Rule-Based Lattice Model

The present model for simulating conductive heat transfer and solidification is based on a 2D cubic lattice. The lattice is contained within a square shape containing 122,500 cells (i.e. 350 x 350). It was assumed that the dendrites were thermal in nature and that in the simulations to be reported the seeds were initially located in supercooled liquid. The model assumes the following rules and conditions;

(a)   liquid sites having a value 0 will transform to solid sites having an integer value. In the case of simulated equiaxed structures each equiaxed grain is identified by a different integer. In the case of columnar structures each primary dendrite arm is similarly identified;

(b)   conductive heat transfer is modelled by upgrading the temperature T_i of every site at each time step in the following manner; the average temperature of the four nearest neighbours surrounding a particular site is calculated and the temperature of the site T_i is then moved in the direction of the average value by an amount governed by an assumed heat transfer constant;

(c)   a site will only solidify if there are more than a given number of solid sites in its neighbourhood;

(d)   growth can only occur if a site temperature $T_i < T_{crit}$;

(e)

$$T_{crit} = \frac{\gamma}{c} \qquad\qquad (2)$$

where γ is a measure of the solid-liquid interfacial energy and c is a measure of the local curvature. An assumed value is used for γ, and c is determined from the number of solid site neighbours which reflects the curvature; as the number of solid site neighbours increases, T_{crit} increases;

(f)   if a liquid site transforms to solid the temperature of that site is raised to a fixed value.

Application of the Model and Observations

The observations to be reported are the result of extensive initial trials to obtain the set of values and start conditions required to implement the above rules and obtain structures having a realistic dendritic appearance.

Two simulations are presented to illustrate the application of the model to the solidification of columnar and equiaxed dendritic grain structures. In both examples the melt is assumed to be initially at a uniform predetermined undercooling. For the columnar grain simulation illustrated in Fig. 1, 100 primary arm seeds (3 x 3 cells in size) were randomly located along the bottom edge. In the equiaxed grain simulation shown in Fig. 2, cube shaped seed crystals (3 x 3 cells in size) were randomly located within the square. In both simulations, at the onset the seeds and melt were at the same temperature. Also, it was assumed that there was no heat loss from the system during the solidification simulations. This was achieved by setting the boundary conditions when modelling the conductive heat transfer so that the top and bottom edges of the square are fully insulating and the side faces are periodic i.e. as if in contact with each other.

The striking feature of the figures is the manner in which oscillatory branching of the dendrites is simulated. In the case of the columnar dendritic structure competitive growth of the primary arms leads to readjustment of the spacing as freezing progresses. In both figures temperatures in the melt are colour coded into three bands. This enables the observer to have a feel for the form of the predicted temperature distribution. Black represents the coolest liquid and the darker of the two lighter colours the hottest.

Summary

The present paper illustrates the fact that rule-based lattice models can be employed to qualitatively simulate the combination of factors that determine the macroscopic shape of a thermal dendrite. As well as supporting our academic understanding of branched thermal dendrites these models can also play a valuable role as educational tools. Although thermal dendrites do not form as columnar structures in practice, the ability to artificially model constrained thermal dendrites by confining nucleation to outer surfaces may also aid understanding of the growth of constrained alloy dendrites.

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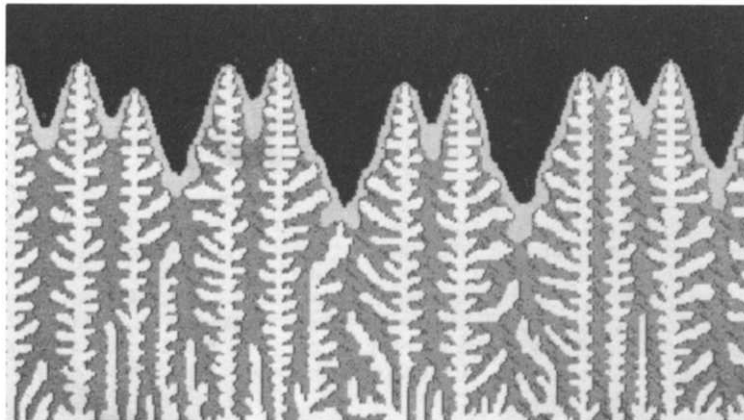19. G. Weisbuch and S. Ryckebusch, Complex Systems Dynamics, p.36, Addison-Wesley, Redwood City (1991).

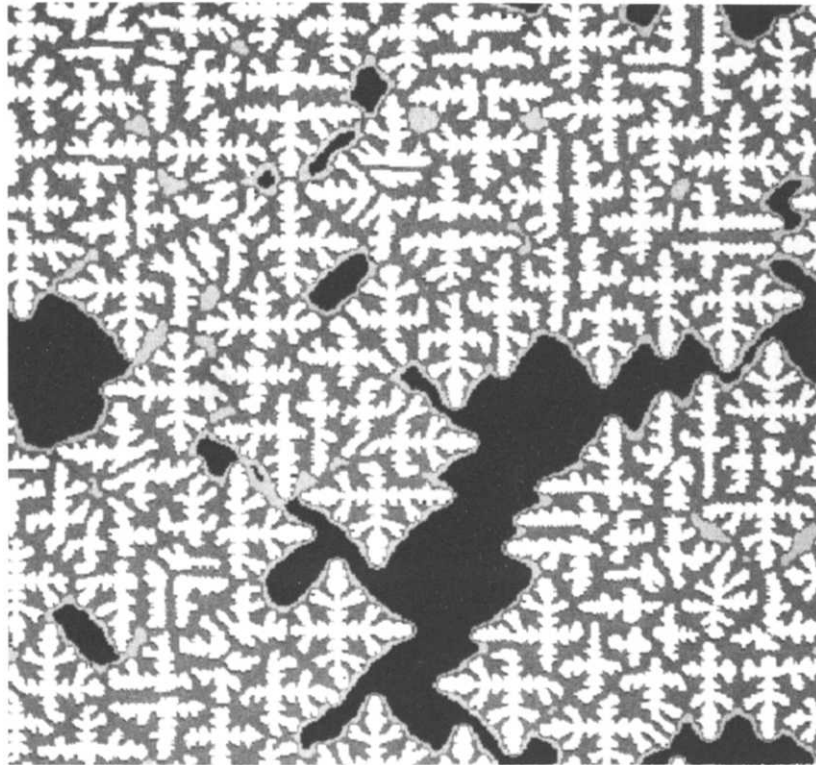FIG. 1. A rule-based lattice simulation of columnar dendritic growth.

FIG. 2. A rule-based lattice simulation of equiaxed dendritic growth.