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A cellular automaton model of steady-state columnar–dendritic growth in binary alloys

J. A. SPITTLE, S. G. R. BROWN
IRC in Materials for High Performance Applications, Department of Materials Engineering, University of Wales Swansea, Singleton Park, Swansea SA2 8PP, UK

A two-dimensional cellular automaton model has been developed to examine the evolution and coarsening behaviour of solid-solution dendrites during steady-state columnar freezing. Using an empirical rule to account for interface growth, realistic dendrite geometries were obtained for different assumed compositions and process conditions. Coarsening occurred by a coalescence mechanism associated with bridging of adjacent dendrite arms.

1. Introduction

Research and commercial finite element/finite difference codes are now well established for the numerical simulation of conductive heat transfer and freezing in alloys for a variety of solidification processes, including casting, welding and directional solidification. Some packages, with limited success, can also handle fluid flow and associated thermal transport prior to and during solidification and, also, include radiative heat transfer. The most widely used commercial packages are those for the modelling of casting processes and several hundred have now been installed worldwide in foundries and research organizations. Consideration of these packages and of examples of their application has recently been the subject of three major surveys carried out in Japan [1], Europe [2] and the USA [3]. Although simulation software holds the potential for the prediction of a whole range of solidification features, including microstructure evolution, segregation and the formation of defects such as pores, current limitations relating to the incorporation of descriptions of microscopic behaviour restrict the application of most packages to the prediction of macrophenomena. Most packages are presently employed to predict the macro-freezing patterns of castings and to identify if isotherms form closed loops around still solidifying volumes. Such isolation gives rise to macroshrinkage defects.

The assumptions in the majority of numerical solidification simulation packages of casting, excluding those that specifically incorporate a micro–macro model of equiaxed growth, imply that freezing occurs in a columnar fashion, irrespective of the composition and freezing range of the alloy, i.e. continuous growth of grains from the mould/die walls in a direction opposite to the principal heat-flow direction. This arises because nucleation is ignored and growth is assumed to commence when the local temperature falls to the equilibrium liquidus value. In alloys that freeze over a temperature range, the primary phase grains are frequently dendritic. Columnar–dendritic growth will only take place in practice in dilute alloys, in the absence of grain refiners, and is encouraged by high pouring temperatures.

Often, however, the dendritic grain structures of the primary phase are equiaxed. Equiaxed grains nucleate and grow in supercooled liquid, the rates at which both occur being temperature dependent. Although so-called micro–macro numerical models of equiaxed grain growth have been reported [4, 5], which couple a macro-heat-transfer model with a micro-model of equiaxed grain nucleation and growth, the models still do not encapsulate the essential aspects of equiaxed grain formation. Spittle and Brown [6, 7] were the first to demonstrate, using a qualitative cellular automaton model, the range of factors that need to be simulated by models in order to predict grain-structure evolution. These include nucleation, solute redistribution on freezing (together with associated grain-growth restriction and melt undercooling), grain and heat transfer due to fluid flow and, grain remelting in superheated liquid.

A major limitation of numerical models of cast alloys solidifying over a temperature range, whether they are of the columnar or equiaxed freezing type, is their failure to simulate directly the solute redistribution on freezing and related microstructural phenomena. Solute redistribution, in conjunction with the solidification conditions, will determine the grain structure of a casting, the scale of the dendrite arm spacing (which in turn will influence interdendritic pore formation and the permeability of the solid + liquid region), the pattern of microsegregation and the amount of eutectic. At the present time, in macro-heat-transfer models, solute partitioning and diffusion during dendritic freezing are not modelled directly. In most commercial software, solute redistribution is dealt with by the incorporation of analytical models, which relate fraction solid to temperature, based on assumed conditions controlling solute transport during freezing. The two most common analytical models, which also define the extreme limits regarding the

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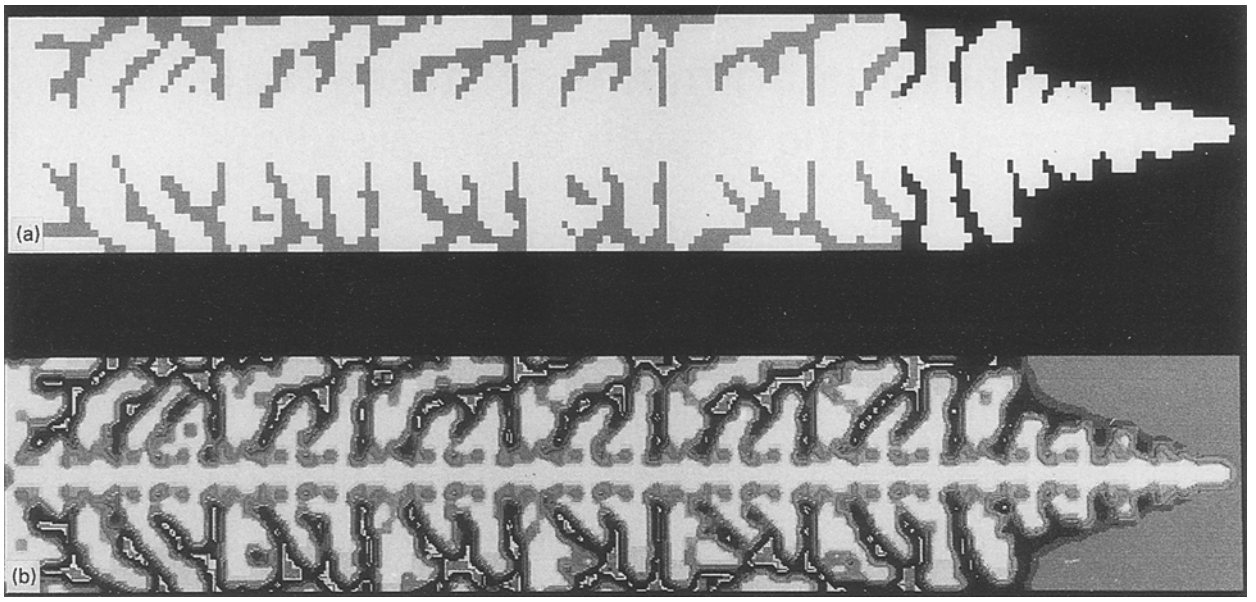

Figure 1 A two-dimensional cellular automaton simulation of steady-state dendritic growth for a hypothetical alloy containing 0.07% solute grown at a reference growth rate with a reference temperature gradient: (a) the dendritic (white), eutectic (grey) and liquid (black) portions, and (b) a microsegregation map.

possible extent of microsegregation, are the equilibrium freezing model and the Scheil model [8]. The first assumes complete solute diffusion in the solid and complete mixing of the liquid throughout freezing, the second assumes no diffusion in the solid and complete mixing of the liquid. Several other analytical models have been developed, representing modifications of the basic Scheil model, which variously take into account "back diffusion" of the solute into the solid during freezing, dendrite tip undercooling and dendritic arm coarsening [9–12].

In the case of current numerical macro-heat-transfer models of columnar–dendritic freezing, a fraction solid versus temperature relationship is often employed to specify the rate of rejection of latent heat at locations throughout the casting. The limitation, of the modified versions of the Scheil solute redistribution model, is that they are unable to anticipate accurately the influences of interface undercooling and back diffusion on solute distribution under conditions where the dendrite structure is continuously evolving and coarsening and where the local solidification conditions are continuously changing.

A number of microscopic numerical models for predicting microsegregation in binary dendritic structures have also been reported [13–16]. These assume that the dendrites have a plate-like morphology and then perform a one-dimensional numerical analysis of solute redistribution between two adjacent secondary arms for different cooling rates. Again, these models cannot simulate the transient conditions in real systems where dendrite morphology and local solidification conditions are continuously changing. Also, they are forced to employ an empirical expression to account for coarsening.

In order to improve the accuracy of the predictions of macro-heat-transfer models of solidification and to enhance microscopic predictive capabilities, better models of columnar–dendrite evolution are necessary which try to simulate the actual manner of evolution of the dendrite array.

There have recently been a number of attempts, employing different modelling procedures, at simulating the complex interactions governing the evolution of dendrites. Some of these have investigated the qualitative modelling of pattern formation during dendritic growth using either aggregation-type models [17, 18] or cellular automata [19, 20]. Others have attempted to produce quantitative models of branched dendrites using phase-field techniques [21] or mixed numerical/empirical approaches [22]. Most of these models have considered the free growth of equiaxed crystals, usually of pure materials, into an undercooled melt. Lu and Hunt [23] have developed a wholly numerical model of unbranched (no secondary or higher order branches) cellular and dendritic columnar growth for the prediction of cell and primary dendrite arm spacings.

The object of this paper is to describe a cellular automaton model of columnar-dendritic growth, developed for the purpose of beginning to investigate dendrite evolution as a function of alloy parameters and processing conditions.

2. A two-dimensional cellular automaton model of steady-state columnar–dendritic growth in binary alloys

The model is based on the authors' previous experience of developing cellular automata models of "free" dendritic growth [19, 20]. The model operates within a regular two-dimensional lattice of square-shaped cells. The lattice domain is rectangular in shape and contains 5425 cells (31×175). Each cell can be identified by one or more variable(s) (in the present instance temperature and composition) and by the state of the cell, namely, primary phase, eutectic or liquid. Growth is initiated from a seed of three cells width, placed centrally along the edge at one end of

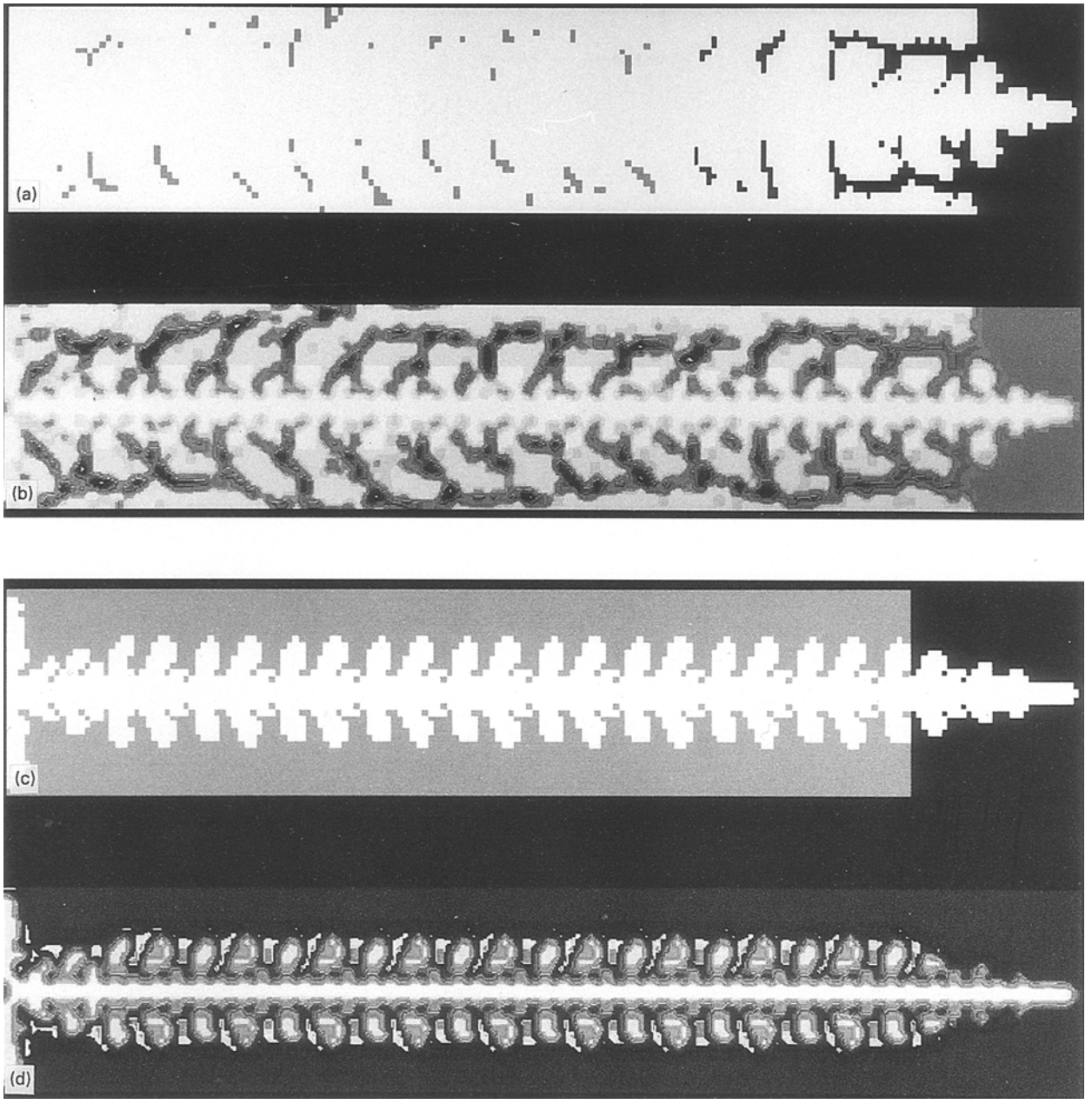

Figure 2 Cellular automata simulations of steady-state dendritic growth for alloys containing (a, b) 0.04% solute, and (c, d) 0.10% solute, using the same growth rate and temperature gradient as in Fig. 1.

the rectangle. The long edges of the rectangle are treated as being periodic, i.e. in contact with each other.

A hypothetical binary eutectic system was examined and it was assumed that the liquidus and solidus lines were straight. The phase diagram characteristics at the solvent end were assumed to be as follows; melting point of solvent 933 K, eutectic temperature 840 K, partition coefficient, k, 0.18, and liquidus slope, m, 650. Steady-state columnar growth was achieved by moving a linear temperature field along the domain in steps. When advancing the temperature field, the line of cells lying two cells ahead of the leading dendrite tip was set to the equilibrium liquidus value for the initial alloy composition under investigation.

Within each temperature-field advancement step the following routines are performed. All liquid sites are checked to determine whether they satisfy the necessary conditions to freeze. For growth to occur, a cell must have $\geqslant 3$ solid nearest neighbours, where each cell has 8 nearest neighbours, and be at a temperature below the liquidus temperature for the cell composition. If a cell freezes, its solid composition for its temperature is calculated and the solute rejected is apportioned uniformly to all its nearest neighbour liquid cells. If the temperature of a cell is less than or equal to the eutectic temperature, the cell will solidify automatically and with no rejection of solute. Following growth and solute rejection, solute diffusion in the liquid was simulated by averaging the composition of each liquid cell with all of its surrounding nearest neighbour liquid cells and then moving the cell composition in the direction of the average value by an amount determined by an assumed coefficient. No solute diffusion was permitted in the solid. Solute rejected on freezing and solute transported by diffusion is not allowed to enter cells ahead of the line of cells corresponding to the position of the leading dendrite tip.

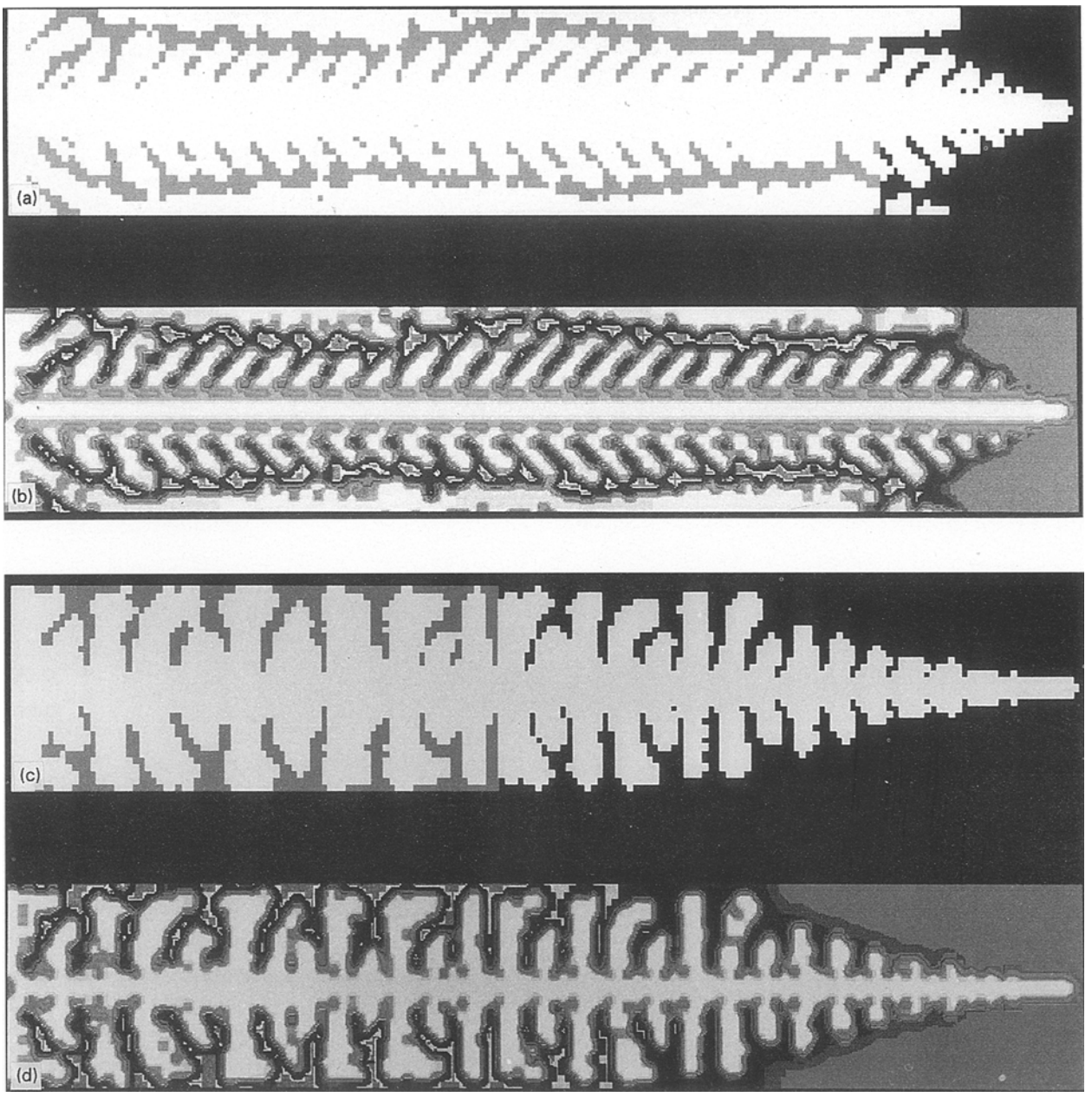

Figure 3 Cellular automata simulations of steady-state dendritic growth for a temperature gradient (a, b) higher and (c, d) lower than in Fig. 1, but with the same alloy composition and growth rate.

Simulation of the possible effects of increasing dendrite growth rate, on dendrite evolution and solute redistribution during freezing, was achieved by varying the number of iterations, n, of the combined growth, solute rejection and solute diffusion routines conducted within each temperature-field advancement step. It was arbitrarily assumed that a smaller number of iterations would correspond to a higher tip-growth rate. In a real system, the faster the rate of advancement of the columnar dendrite tip the less time would be available for solute diffusion in the interdendritic liquid regions.

Alloy compositions and temperature fields were selected that enabled the temperature within the domain to fall to the eutectic temperature and which provided sufficient distance within the domain length for the establishment of a steady-state freezing condition.

3. Model simulations

The above model has been used to provide an insight into the influences of alloy composition, temperature gradient and growth rate on the evolution of columnar–dendrites in binary alloys under steady-state freezing conditions. Because the cells do not correspond to an actual physical size and because no time-dependent equations are being solved, actual temperature gradients and growth rates cannot be specified. Likewise, the arm spacings in the simulated dendrites cannot be measured in real dimensions.

The results of each simulation are illustrated in two forms. The first illustration shows the regions of the domain that are liquid (black), primary dendrite phase (white) and eutectic (grey) at the instant when the dendrite tip reaches the end of the domain. The second provides a contour map (micrograph) of the solute distribution in the alloy at the same time. The

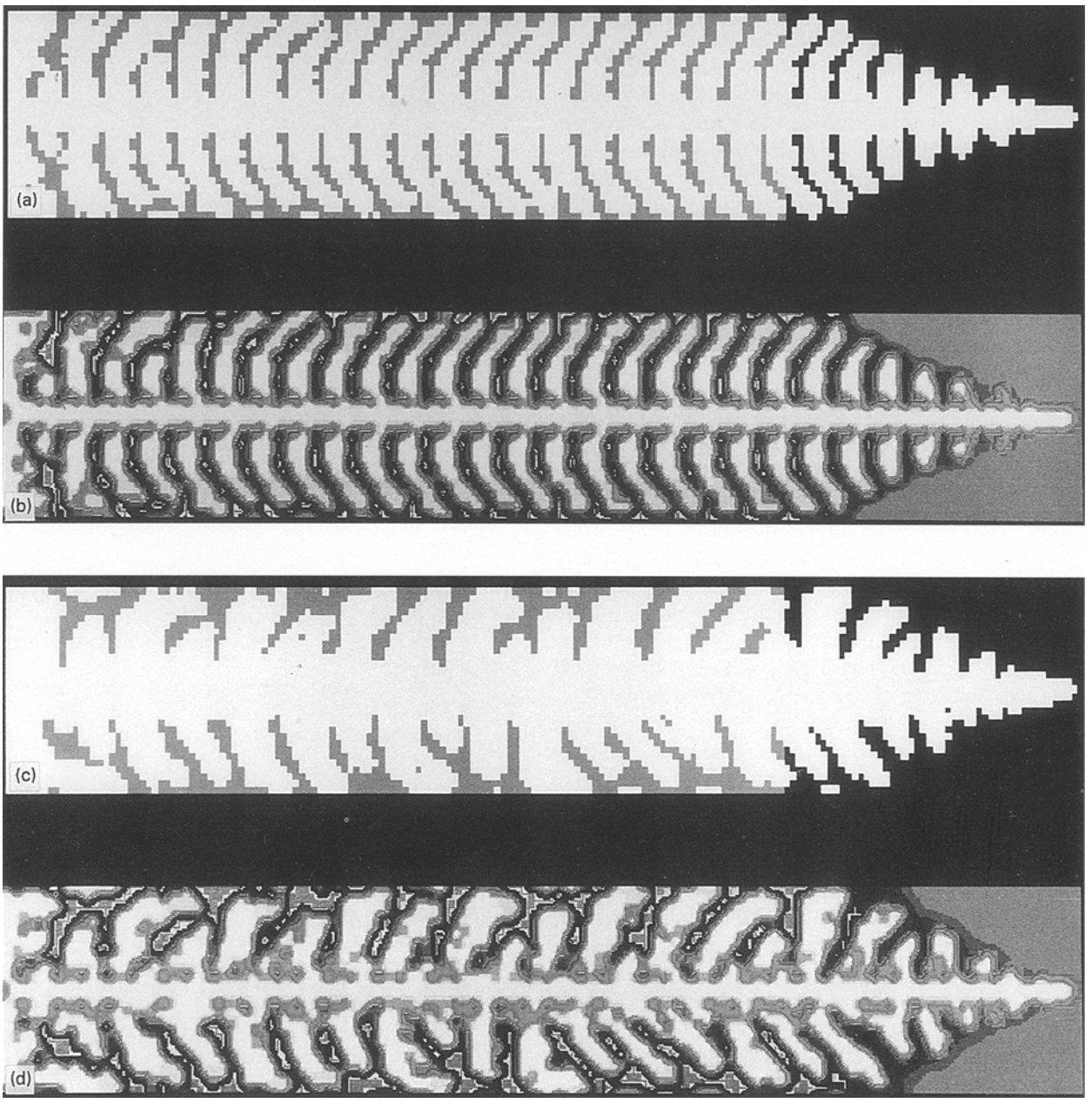

Figure 4 Cellular automata simulations of steady-state dendritic growth for a growth rate (a, b) higher and (c, d) lower than in Fig. 1, but with the same alloy composition and temperature gradient.

dendrite core of low solute content is readily recognized.

A reference simulation, representing an intermediate composition (0.07%), growth rate and temperature gradient, against which the individual effect of each of the three variables was assessed, is shown in Fig. 1. Temperature gradients and growth rates greater or less than those in Fig. 1 are simply referred to as high or low, respectively.

Fig. 2a–d illustrate simulations for compositions of 0.04% and 0.10%, respectively, for the same gradient and growth rate as in Fig. 1. As can be seen, with increasing solute content the amount of primary phase in the alloy decreases, the non-equilibrium freezing range decreases and the dendrites are more rod-like. This conforms with actual observations. By comparing Fig. 2a and b, the dendrite coarsening mechanism by coalescence can be appreciated. This mechanism has been discussed by Young and Kirkwood [24]. As growth proceeds, individual arms thicken and eventually adjacent arms can coalesce with the entrapment of solute material previously present at the base of the dendrite arms. It can be seen from Fig. 2a and b that a tertiary arm has continued to grow as a primary, which is a recognized mechanism of primary spacing refinement. The general observations from Figs 1 and 2 that secondary arm spacings tend to decrease and primary arms increase with increasing solute content, conforms with experimental observations [25] and theory [26], respectively.

Fig. 3a–d illustrate the effect of high and low gradients for the same composition and growth rate as in Fig. 1. Again we have a situation in Fig. 3a and b where a tertiary arm has become a primary. Again the finer spacings for the secondaries and primaries with increasing gradient conform with experiment [25] and theory [26], respectively. For the same composition and growth rate, increasing the gradient will

decrease the local solidification time, i.e. the time available for secondary arm coarsening.

Fig. 4a–d illustrate the effect of high and low growth rates for the same composition and gradient as in Fig. 1. The finer secondary arm spacing observed at the highest growth rate again conforms with experimental observations and also corresponds with a reduction in the local solidification time. The observations also give support to the method adopted in the model for simulating variations in growth rate.

4. Discussion

Remarkable success has been achieved, with a relatively simple cellular automaton model, in demonstrating many of the features of columnar (array) dendrites in real systems grown under steady-state conditions. The influences of composition, temperature gradient and growth rate on arm spacings and dendrite morphology agree extremely well with reported experimental observations and theoretical predictions. The model emphasizes the importance of the amount of primary phase in the alloy and the local solidification time on the evolving dendrite morphology. The model illustrates secondary dendrite arm coarsening by coalescence (as opposed to remelting) which is a mechanism that a number of researchers have postulated. Although it is not quantitative, the model provides a valuable insight into the complexity of dendrite structure development and the problem associated with attempting to describe the evolution of the fraction solid in dendrites using analytical methods. The problem is further exacerbated by the fact that columnar dendrites in real castings grow under transient growth conditions. Work is at present proceeding to try to enhance the physics of the model by incorporating actual length scales and the transient time-dependent equation for solute diffusion.

5. Conclusion

A two-dimensional cellular automaton model has been developed to simulate steady-state columnar–dendritic growth in binary alloys. The predictions of the influences of composition, gradient and growth rate on dendrite arm spacings and morphology are in excellent qualitative agreement with experimental observations and theoretical predictions. The model emphasizes the importance of the further investigation of procedures for the simulation of microstructural evolution during solidification.

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