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A computer simulation of the influence of processing conditions on as-cast grain structures

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A computer model for simulating solidification and involving a Monte Carlo procedure has been used to qualitatively predict the influence of solidification conditions on the grain structures of small castings. In agreement with experimental observations, it was found that increasing either superheat or mould temperature results in coarsening of the grain structure. This agreement supports the contention that the principal mechanism of equiaxed grain formation in small castings is heterogeneous nucleation. The model also illustrates the importance of simulating equiaxed grain movement in the bulk liquid in order to obtain realistic predictions of grain structures.

1. Introduction

In a recent paper [1] the authors presented a Monte Carlo computer technique for the simulation and pictorial representation of grain growth and macrostructure development during the solidification of castings. The model simulated the hypothetical case of the nucleation and growth of static grains of uniform composition in an isothermal system. It was shown, by predetermining the number, location and time of origin of grain nuclei, that all types of grain structure observed in uni- or omnidirectionally solidified castings could be simulated. The technique also permitted the determination of the physical state leading to a columnar to equiaxed grain transition, namely the volume fraction of equiaxed grains ahead of the columnar interface at the transition.

The preliminary study outlined above [1] was intended to introduce the Monte Carlo technique as a method of simulating and enhancing the understanding of liquid to solid phase transformations. Previously, the method has been used to simulate various aspects of microstructural evolution in the solid state [2–6].

The initial model for simulating solidification [1], though successful, was limited in that it was only able to provide a simulated description of the macrostructures that are possible in castings based on an assumed pattern of nucleation behaviour. No account was taken of heat transfer from the solidifying system, latent heat of fusion, movement of equiaxed grains in the bulk liquid, nuclei remelting and solute redistribution during solidification. Therefore, the model was not in any sense intrinsically predictive since it was unable to anticipate the influence of casting conditions, phase diagram characteristics or the physical properties of the system on the nucleation and growth processes.

The Monte Carlo model presented in this paper represents an attempt to create a model that is able to qualitatively predict the grain structures of small castings. This has been achieved by including procedures to take into account heat conduction, equiaxed grain movement in the bulk liquid and nuclei remelting together with accompanying latent heat absorption. It should also be noted that the simulation commences as an "empty box" which corresponds to a completely liquid state. As the thermal conditions change in the system, so the nucleation and growth processes naturally proceed i.e. no assumptions are necessary regarding the pattern of nucleation behaviour.

Although recognizing that solute content and phase diagram characteristics have major effects on as-cast microstructures and grain structures, these variables are not incorporated at this stage. The present model therefore equates to a situation where a melt of given composition is poured into a mould of fixed dimensions. As heat is lost from the system, solidification proceeds by nucleation and growth of grains of uniform composition corresponding to that of the melt. This model should therefore permit the prediction of the effects of superheat and mould temperature on cast grain structure. Experimental studies have been made on small castings to examine the variation of grain structure with superheat [7] and mould temperature [8]. The influences of these parameters are therefore known and accepted and allow comparisons to be made with the model predictions.

2. Solidification simulation model

As previously reported [1], the solidification simulation procedure involves the use of a two dimensional lattice consisting of 10 000 lattice sites arranged in a triangular lattice pattern. The form of the arrangement of the sites is shown in Fig. 1 for a portion of the lattice. The sites are located within a square shape, the length of each side corresponding to 100 sites.

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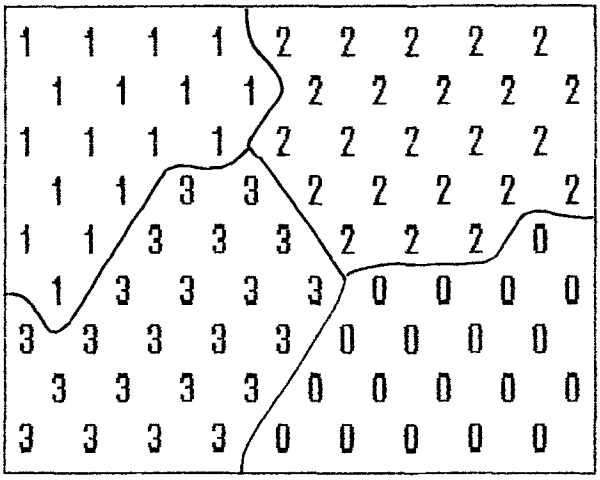

Figure 1 A portion of the two dimensional lattice used in the model.

Initially, every lattice site is assigned a number P equal to 0 indicating that each site is liquid. During the course of simulated solidification, sites that are liquid will transform to solid. This is indicated by a change in site value to a P number > 0. All sites within the same grain have the same P value and the total number of P values that survive (in the range $1 \rightarrow Q$) represents the number of grains in the finally solidified simulated casting. It is assumed that the square shape represents the cross-sectional structure seen along the length of a plane lying parallel to and containing the long axis of symmetry of a cylindrical casting i.e. columnar grains, if present, only grow from one pair of opposite sides of the square.

In addition, each site is ascribed a value T denoting the particular temperature at each site. Initially, in each simulation, the outermost layer of sites adjacent to the left and right hand sides of the square was assigned a specific value of $T < T_{\text{Liquidus}}$. This value simulates the mould temperature. T_{Liquidus} represents the T value chosen for the liquidus temperature. All the remaining sites were assigned a value of $T > T_{\text{Liquidus}}$ corresponding to the temperature of the superheated melt.

Solidification simulation proceeds by a sequence of steps each step being comprised of three modelled stages, namely thermal conduction, nucleation and growth.

Heat conduction from the system is simulated by averaging the temperature of every site with its nearest neighbours and resetting each site value to the averaged value. After resetting all the values, the outermost layers of sites on the left and right hand sides are returned to their initial value i.e. the mould wall temperature is maintained at a constant value throughout solidification.

After the heat condition routine, the temperature of every lattice site is sequentially measured. If $T < (T_{\text{Liquidus}} - x)$, where x is the undercooling for nucleation, nucleation can occur resulting in the formation of a rhombus shaped 4 site nucleus. Any nuclei incorporating sites in the layer adjacent to the sides of the square remain where they are to act as possible nuclei for columnar grain growth. Potential nuclei created outside this layer are immediately randomly relocated on the lattice. However, the nuclei will only actually form provided that the randomly selected position consists of all liquid sites. If the randomly selected position has any solid present the nucleus will not form. This random relocation simulates movement of grain nuclei due to convection in the bulk liquid.

Following nucleation and relocation of nuclei, remelting or growth of grains is simulated. A site is randomly selected and tested for its P and T values. If $T \geqslant T_{\text{Liquidus}}$ and $P > 0$ the site will transform to $P = 0$. The temperature of the site will also change from T to $(T - y)$, where y is the temperature drop at a site associated with latent heat absorption on remelting. Simulating latent heat absorption helps to reduce the bulk liquid temperature which, in reality, occurs mainly by melt convection. If the randomly selected site is liquid and if the temperature of the site is $< T_{\text{Liquidus}}$ the site may solidify. To determine whether or not the site will solidify employs the following procedure, which has been described previously [1].

The energy associated with a solid–liquid interface is set by considering the interaction between nearest neighbour sites [2] using

$$H = -J \sum_{nn} (\delta P_i P_j - 1) \qquad (1)$$

where P_i is the P value on site i and δ_{ij} is the Kronecker delta. If $P_i = P_j$, $\delta = 1$ and if $P_i \neq P_j$, $\delta = 0$. The sum is taken over all nearest neighbour sites nn ($nn < 7$). A nearest neighbour pair is therefore associated with an energy J if the two sites are of unlike P value and with zero energy if alike. The summed energy, H_0, of the randomly selected site, considering all nearest neighbour interactions with the site is calculated using Equation 1. The P value of the site is then randomly changed to a P value of one of the nearest neighbour sites and the new summed energy, H_n, determined. The change in energy accompanying this site change, ΔH, is given by

$$\Delta H = H_n - H_0 \qquad (2)$$

If ΔH is positive or zero the site remains in its original state. However, if ΔH is negative the new value of P is retained. Site changes at an interface correspond to interface movement. In order to ensure that solidification proceeds at a solid–liquid interface and not remelting, the site randomly selected, whether before or after its P value is randomly changed, is given an additional energy increase of H_L if $P_i = 0$; i.e.

$$\left.\begin{aligned} H_0 &= H_0 + H_L \\ \text{and} \quad H_n &= H_n + H_L \end{aligned}\right\} \text{if } P_i \text{ of selected site } i = 0 \qquad (3)$$

Liquid sites therefore have an intrinsically higher energy than solid sites.

The procedure of randomly selecting a site to determine if the site will remelt or freeze was repeated 10 000 times before proceeding to the next heat conduction stage.

The value of J was taken as 1 and the value H_L taken as 3. These values guarantee that a liquid site will only change to a solid site if it has at least two

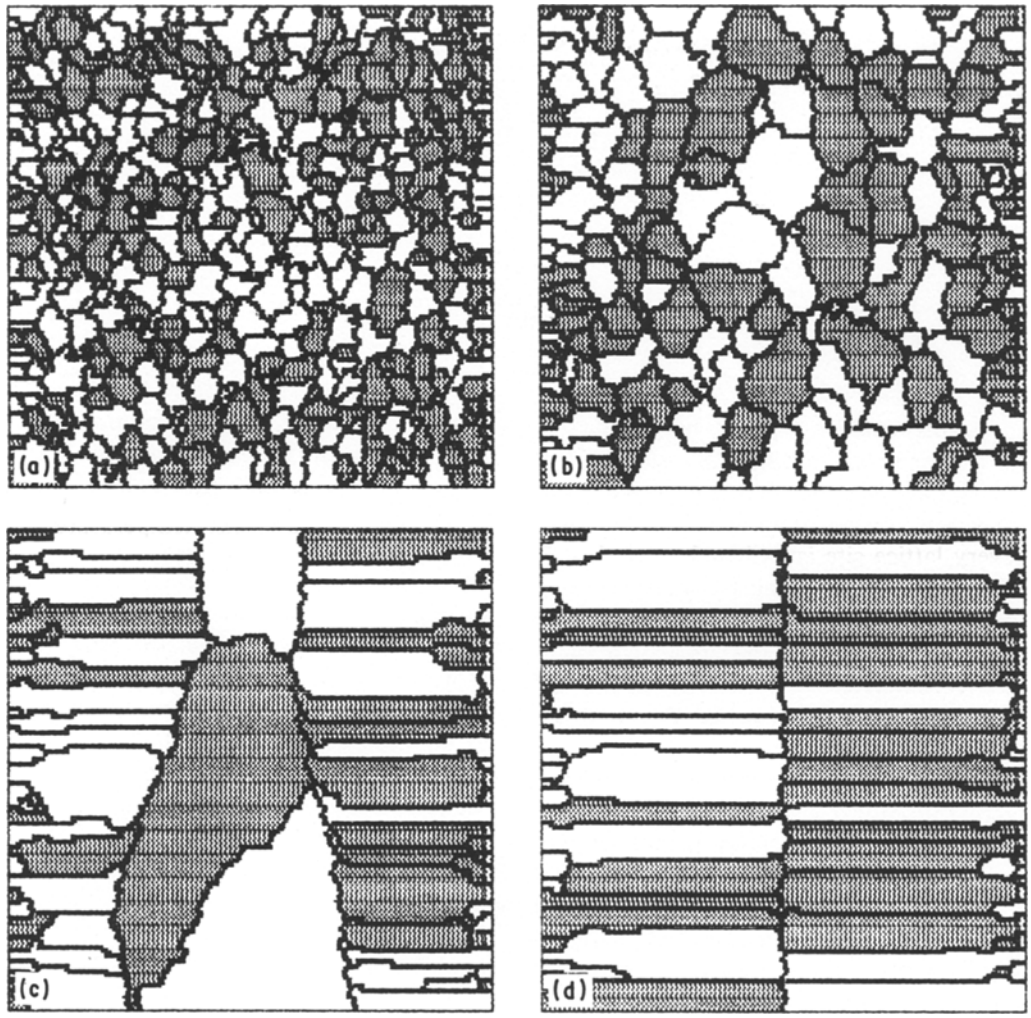

Figure 2 Computer simulated macrostructures for modelled superheats of (a) 0.005, (b) 0.02, (c) 0.04 and (d) 0.05.

neighbouring grid sites which are solid. This produces realistic grain shapes and macrostructure development.

Another feature included in the growth routine was equiaxed grain pushing. This was introduced as an additional method of simulating equiaxed grain movement in the bulk liquid as an aid to preventing premature columnar to equiaxed zone transition. If any columnar grain comes into contact with an equiaxed grain, the latter is immediately displaced away from the interface one nearest neighbour spacing. This can only happen provided the equiaxed grain does not make contact with another equiaxed grain.

In the model outlined above the permitted processing variables are superheat and mould temperature.

3. Simulation trials

Since the above model does not consider the influence of composition or of phase diagram characteristics on the macrostructures of castings, it might be thought that the model simulates the structures of both pure metals and alloys freezing over a temperature range. However, for the reason that follows, the simulated macrostructures more realistically reflect the effects of casting conditions on solid solution grain macrostructures. It is widely accepted, for small castings, that the grain nuclei are formed in the early stages of freezing [9, 10]. The superheat is quickly lost due to convection and pouring turbulence and those nuclei that are in suspension in the bulk melt will only be able to survive remelting and continue to grow as equiaxed grains provided that they find themselves in supercooled liquid. Constitutional supercooling in the bulk melt, ahead of the advanced columnar interface, can occur in alloys freezing over a temperature range but not in pure metals. The macrostructures of pure metal castings are therefore columnar because the nuclei cannot survive remelting. In the above model supercooling in the bulk melt results from the simulation of heat conduction and of latent heat absorption when nuclei are remelted, not from constitutional effects. In the following trials, it is implicit that the observations relate to the influence of casting conditions on solid solution macrostructures.

3.1. Effect of superheat

It is commercially and scientifically recognized that increasing superheat results in coarsening of the macrostructures of castings consisting of dendritic solid solution grains. In the case of small ingots, at very low superheats the grain structures are frequently wholly equiaxed. It has often been demonstrated, [11], that with increasing superheat the size of the columnar zone increases and, at the same time, in the central equiaxed zone the number of equiaxed grains decreases and the equiaxed grain size increases. Therefore, an increase in superheat leads to an overall decrease in the total number of grains in the casting. Several mechanisms have been proposed to explain the origin

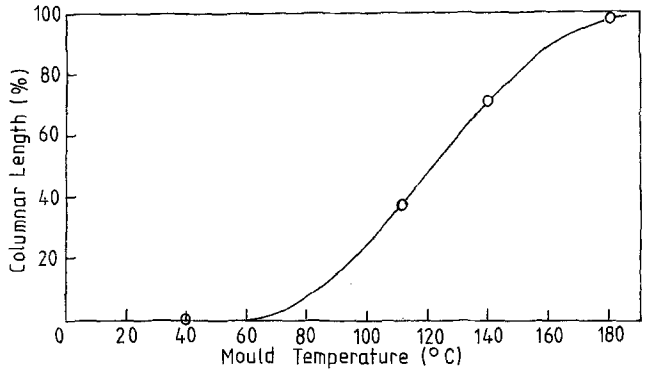

Figure 3 Variation of columnar length with iron mould temperature for Al–5 wt % Cu cast with a superheat of 120° C. Reference [8].

of equiaxed grains invoking either heterogeneous nucleation [7, 12] or dendrite fragmentation [13, 14]. Thermal analysis data [9] and experiments designed to control convection during solidification [10] have demonstrated that the grains constituting the casting are nucleated at the time of pouring. Other experiments [8, 15] have led to the general acceptance that the majority of grains in the equiaxed zone of a small casting originate from heterogeneous nucleation in the supercooled chilled liquid on pouring, the so called "big bang" theory [7].

Convection plays a significant role in determining the final macrostructure by aiding the removal of the superheat and transporting nuclei into the bulk liquid. A number of investigators have shown that reducing convection results in structural coarsening and prolonged superheat retention in the bulk material [10, 16]. Assuming that equiaxed grains originate by the big bang mechanism, increasing superheat will decrease the number of grains initially nucleated (by reducing the extent of the supercooled region on pouring) and increase the probability of nuclei remelting. This will result in a lower density of equiaxed grain nuclei and a consequent increase in columnar grain length.

In the solidification simulations using the model outlined in Section 2, T_{Liquidus} had a numerical value of unity. In examining the effect of superheat, the mould wall temperature used was 0.2 in all cases. The sequence of computerized macrostructures in Fig. 2a–d, which corresponds to selected superheats of 0.005, 0.02, 0.04 and 0.05 respectively, clearly illustrates macrostructure coarsening with increasing superheat. A particularly pleasing feature of the simulations is the realistic increase in columnar length as the structure coarsens. Recently, finite difference models have been used to investigate the influence of a number of variables, including superheat, on the extent of the columnar range [17, 18]. In these models, static equiaxed grain nuclei were introduced into the bulk material either by placing a fixed density of nuclei in the melt ahead of the columnar front or by incorporating into the model a temperature dependent nucleation rate ahead of the columnar front using a heterogeneous nucleation expression. It was found, unlike in practice, that the effect of superheat was negligible and small columnar ranges were predicted for all superheats. The investigators attributed this failure firstly to the fact that the models do not consider big bang nucleation nor the influence of superheat on chill nuclei survival. Secondly, it was recognized that the models did not account for the influence of equiaxed grain movement due to buoyancy and convection.

3.2. Effect of mould temperature

Data relating to the influence of mould temperature on the macrostructures of castings are more scarce since, experimentally, it is less easy to manipulate. However, it has been demonstrated, as seen in Fig. 3, that increasing mould temperature leads to coarsening of the grain structure [8]. The explanation given was that higher mould temperatures like higher superheats make it less likely that big bang nuclei will survive remelting.

In the computerized simulations to illustrate the effect of mould temperature a constant superheat of 0.03 was employed. A series of simulations for mould temperatures of 0, 0.1, 0.25 and 0.5 are shown in Fig. 4a–d. The modelled results are clearly consistent with the experimental data in Fig. 3.

4. Discussion

An earlier Monte Carlo model for simulating grain growth during solidification [1] has been developed to include techniques to account for heat conduction, nucleation, equiaxed grain movement and nuclei remelting during solidification. This has resulted in a model capable of qualitatively predicting the general effects of superheat and mould temperature on the macrostructures of small castings of alloys freezing over a temperature range. The model cannot be applied to simulating the solidification of an alloy in a specific alloy system because it is not based on the use of actual physical properties of a material. Nevertheless, the simulated effects of superheat and mould temperature are consistent with experimental observations. The model is therefore a possible aid to understanding the mechanism of equiaxed grain formation and of the columnar to equiaxed transition. As mentioned earlier, suggested mechanisms for equiaxed grain formation fall into two categories, those involving heterogeneous nucleation and those which rely on dendrite fragmentation. Since no fragmentation can occur in the present model, the solidification simulations support a heterogeneous nucleation mechanism of equiaxed grain formation. As was demonstrated in the earlier model [1], in which different densities of static equiaxed grain nuclei were randomly placed throughout the lattice, only short columnar grains were obtained even at low densities of nuclei. This illustrates the importance of

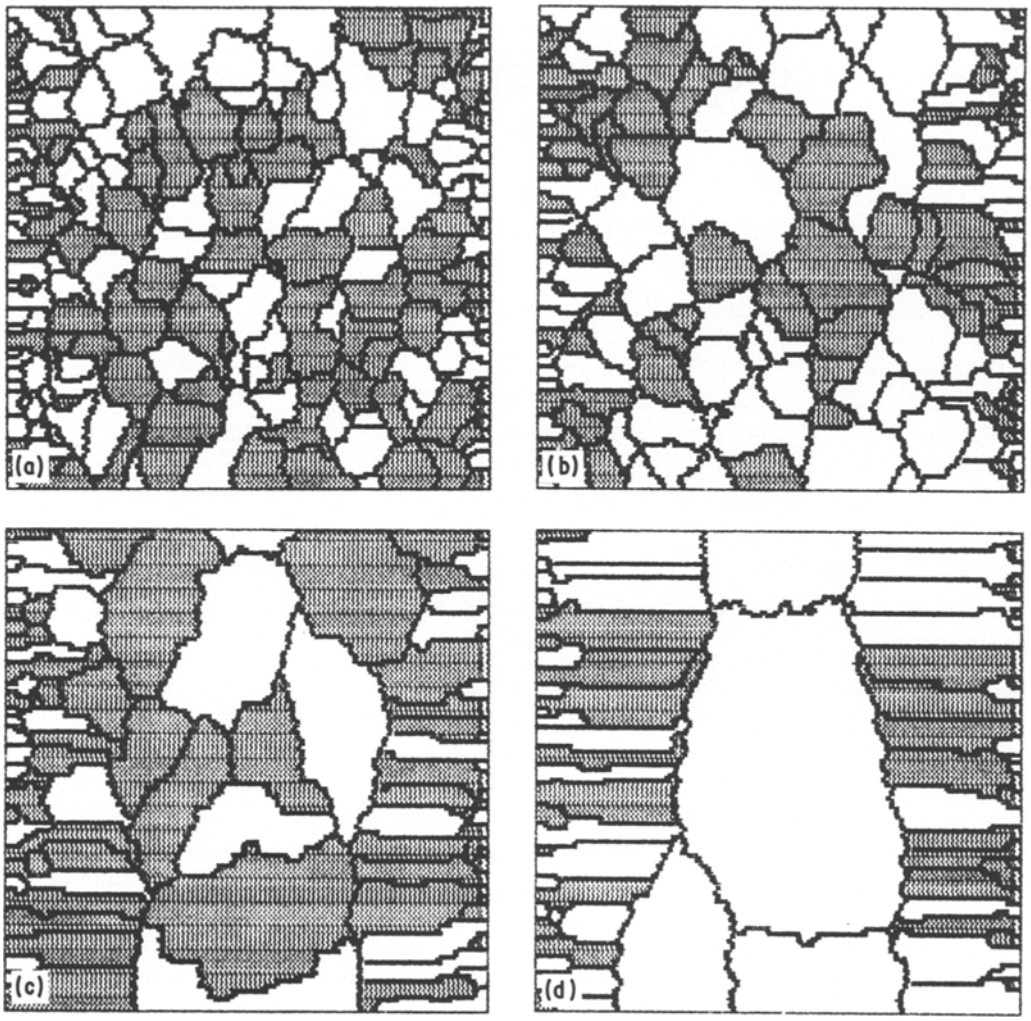

Figure 4 Computer simulated macrostructures for modelled mould temperatures of (a) 0, (b) 0.1, (c) 0.25 and (d) 0.5.

convection and buoyancy to equiaxed grain movement and structural control. In the earlier model it was shown that the columnar to equiaxed transition occurs when the volume fraction of equiaxed grains immediately ahead of the columnar front reaches 0.50.

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