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COMPUTER SIMULATION OF MICROSTRUCTURES

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COMPUTER SIMULATION OF MICROSTRUCTURES

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I

Many phenomena in physical and biological science are governed by the manner in which space is subdivided into discrete elements, "grains" in the microstructure of solid bodies or "cells" in the structure of biological organisms. The topological properties of these divisions may be complex, and few relevant descriptive theorems are known which accurately treat the geometrical properties of real microstructures. However, since the physical processes which generate microstructure are often known, the geometry of microstructure can be studied through direct computer simulation.

In metallurgical systems the microstructure is a grain structure often generated through a nucleation and growth process. During the phase transition which establishes the grain structure small nuclei of the new phase form within the matrix of the old and grow until they impinge and fill space. The research reported here addresses the computer simulation of those processes and the characterization of the resulting grain structures.

Our initial project is a simulation of the Johnson-Mehl grain structure (1). Two parameters control the generation of this structure: 1) the nucleation rate, N, which is constant and equal to the number of nuclei formed, per unit volume per unit time and 2) the linear growth rate, G, which is assumed constant and isotropic. Nucleation is a random process and the transformation involves a simple change of phase, for example, a change of crystal structure. In the transformation spheres nucleate at random sites as a function of time and grow until impingement. It is assumed that no further grain growth occurs after this impingement; first impingement surfaces define the grain boundaries. The division of space which results from such a process is called a grain structure of the Johnson-Mehl type.

In the computer simulation the grain structure is examined by taking a series of slices along the z-axis of the transformed body. The resulting two-dimensional microstructures are then drawn (for example, Figure 1). The analogy would be a series of polished planes from a real crystal structure. These two-dimensional "surfaces" are then characterized geometrically. The geometrical measurements are obtained within the program in two ways: 1) by direct measurements of the microstructure and 2) by simulation of quantitative techniques used in the experimental analysis of real microstructures such as the Rhines Area Tangent Count (2) and the intersection method (3). Since the Johnson-Mehl model is well-defined, it provides a basis for correlation between the creation parameters and the resultant microstructure.

Normal characterization of a microstructure involves the characterization of shape (4). Measurements are made of the mean and distribution of grain size, the number of sides per grain, the angles of intersection at a node (three side junction), and the curvature of the sides or interfaces. Extrapolation of these results yields a three-dimensional statistical description of the grain structure. Similar measurements may be made on real microstructures by "serial sectioning" techniques, (5) however it is not now possible in experiment to infer the processes controlling the generation of shape from the geometric characteristics of the final microstructure. Using computer simulation this correlation is straightforward.

In the simulation, the nucleation and growth parameters are input data. The computer data is threefold. A table is generated describing the time at which a given site nucleates and the grain growth rate from that site. (This latter piece of information will become important when the growth rate is varied as a function of several parameters.) The microstructure of a chosen z-plane can be drawn. The computed geometric information about the morphology of the grain structure can be outputed. The input and output data can be correlated statistically and compared to analytical solutions. Our intention is to fully characterize the Johnson-Mehl model before proceeding to more complex microstructures.

In reality, both nucleation and growth are complicated functions of several thermodynamic and kinetic parameters (6). The expansion of the Johnson-Mehl nucleation and growth constants to functions of several parameters is within our present capabilities. Sometimes the grains differ in composition or phase and distinct nucleation and growth parameters may be specified. Subsequent metallurgical phase changes of the nucleation and growth variety will subdivide the specimen again. The new nucleation is frequently confined to old grain boundaries. The results of one division of space problem hence become the input into the next. By solving the Johnson-Mehl model, we produce the framework for the analysis of more complex evolutions, such as may occur in real metallurgical processes.

II

Choosing nucleation and growth parameters and creating a table describing a random three dimensional microstructure is not difficult. However, drawing high resolution two dimensional microstructures of the corresponding three dimensional microstructure in reasonable computing time requires an efficient computing algorithm.

The method for creating a table describing a random three dimensional microstructure is as follows. Given nucleation and growth parameters, random times (ordered) and random sites can be generated using a pseudo random number generator. These sites are generated until the first grain occupies the entire volume implying no sites exist for further nucleation. Each site generated is examined to determine whether it occurred in unoccupied space (valid sites) or occupied space (phantom sites). The later are excluded from the table.

The picture drawing algorithm is now described. Our pictures consist of large bit arrays, e.g., 1024 bits by 1024 bits. On bits (1's) represent boundaries. A picture in this form can be analyzed for various parameters, i.e., area, number of sides, shape factors, etc. Given a table describing all valid nucleation sites (x, y, z; time phase, growth function) we can choose a z plane for our two dimensional picture. Periodic boundary conditions are assumed in all three directions.

A simple brute force solution to this problem is now presented. Divide the selected z plane into 2^{20} subregions (1024 × 1024). For a given subregion, determine what grain impinges first (t_1^S). Determine at what time impingement finishes (t_1^F). Next, determine all other t_i^S. If any t_i^S, $i \neq 1$, occurs before t_1^F then impingement occurs in this subregion. Clearly, if computing time were not important this method could be repeated for all subregions and a valid picture would be constructed.

Next consider a method for improving this brute force algorithm. Consider a z plane consisting of 1024 × 1024 subregions. Next consider a binary tree where the zero node represents the entire z region (plane). Let the nodes at level 1 represent the two subregions defined by bisecting the total region in the x direction. Let the nodes at level 2 represent subregions of the level 1 subregions defined by bisecting in the y direction. Continue construction of this tree until nodes represent subregions of the desired resolution (for example the tree has $20 = \log_2(1024)^2$ levels).

Next consider an arbitrary node (subregion) of this tree. t_1^S and t_1^F can be calculated for this subregion. All other t_i^S, $i \neq 1$, may be calculated. All t_i^S, $i \neq 1$, that occur before t_1^F may impinge in this region, all others do not. Therefore all subregions of the subregion presently being examined need only consider the grains that are candidates for impingement. Furthermore, if no impingement occurs for the present subregion, then obviously no impingement occurs in subregions of the present subregion. Thus nodes below this node do not need to be examined.

By using this technique the binary tree may be searched left to right and top to bottom. The number of comparisons is reduced at lower levels by the screening done at parent nodes. A further reduction occurs because the majority of lower level nodes are not searched. When a lowest level node possesses impingement the appropriate location in a binary array is set to one. The number of comparisons is reduced by several orders of magnitude and thus high resolution pictures become reasonably computable.

A picture post processor is then used to analyze the two dimensional microstructure for area, boundary, curvature, shape and various other distribution functions. In this manner information about the resulting microstructure can be compared with the corresponding creation parameters. Stereology studies are done by examining successive microstructure planes (Fig. 1). Thus we are in a position to verify existing Johnson-Mehl microstructure assumptions and formulate new relationships.

ACKNOWLEDGMENT

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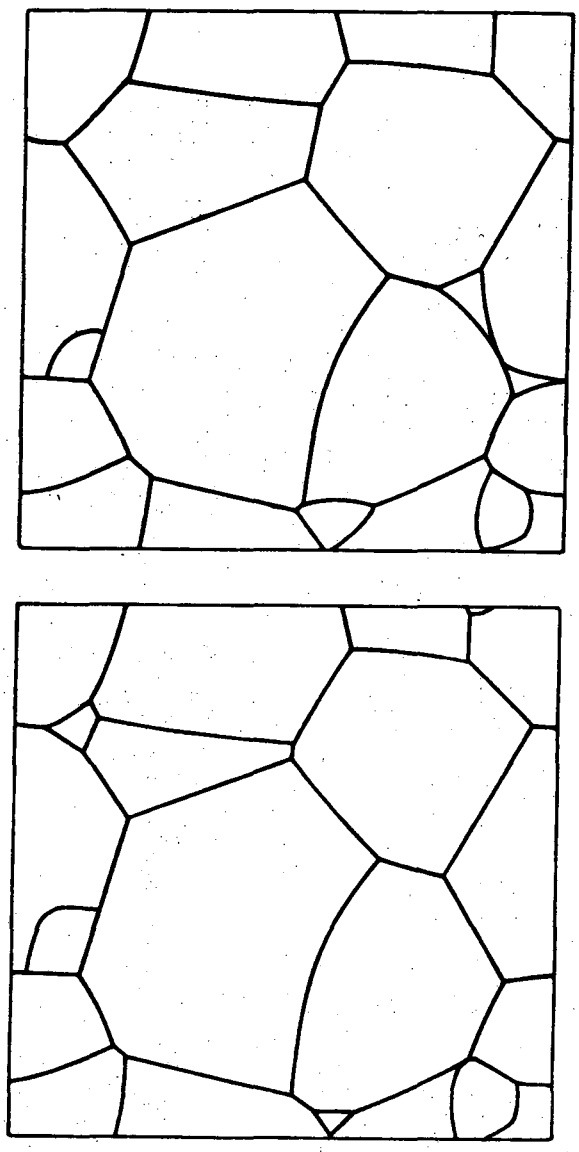

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Figure 1

Successive planes of a computer generated Johnson-Mehl microstructure.

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