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To be presented at the Computer
Simulation Conference, San Francisco,
CA, July 21-23, 1975

LBL-3554
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COMPUTER SIMULATION OF MICROSTRUCTURES

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December, 1974

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48

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COMPUTER SIMULATION OF MICROSTRUCTURES

by

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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.

The specific problem we are investigating is solid state microstructure transformations in metals which proceed through nucleation and growth of new metal grains from the matrix of the old. The nucleation sites can be random or semi random, i.e., preferred nucleation sites such as boundaries of the previous structure. Nucleation times may vary. Once a site is nucleated it is allowed to grow until it impinges on other growing cells. The boundary between cells (microstructure) is defined by this impingement.

Nucleation can be a function of time, space, and phase. Growth can be a function of time, distance, direction, and phase. It should be obvious that very complex three dimensional microstructures can be

obtained by varying nucleation and growth parameters. Our present computer simulation is capable of efficiently creating two dimensional high resolution (million bit) pictures of these complex three dimensional structures. This presentation is concerned with data structure techniques that enable picture construction in reasonable computing time.

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 cell impinges first. 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.

Now we consider methods for improving the brute force algorithm described above. Consider a z plane consisting of 1024×1024 subregions. Next consider a binary tree where the zero node represents the entire z region. 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 z represent subregions of level 1 subregions defined by bisecting in the y direction. Continue construction of this tree until nodes

represent subregions of the desired resolution (for this example the tree has $20 = \log_2(1024)^2$ levels).

Next consider an arbitrary node (subregion) of this tree. t_i^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 occurs 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 cells 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 posses impingement the appropriate location in a binary array is set to one. The number of comparisons is reduced by many orders of magnitude and thus make high resolution pictures reasonably computable.

The generality and efficiency of this procedure enables complex three dimensional structures to be examined. In metallurgy, microstructures influence mechanical properties of metals. Exploring the various nucleation and growth parameters that influence microstructures promises to yield important fundamental theories.

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