THREE-DIMENSIONAL ANALYSIS OF CELLULAR MICROSTRUCTURES BY COMPUTER SIMULATION

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A central problem in Physical Metallurgy concerns the manner in which the properties of a material are determined by its microstructure. While average microstructure parameters such as average grain size are easily obtainable and often correlated with observed mechanical properties it is difficult to parametrize and assess the importance of precise three-dimensional microstructural morphologies. Given the complexity of the microstructure of real materials it is not at all obvious that a useful descriptive parameterization exists.

While many of the interesting geometric properties of a microstructure emerge from an analysis of planar sections, others can only be obtained from a full three-dimensional characterizarion. Examples include the distributions of volumes, surface areas, edge lengths, and numbers of contacting neighbors, the distribution of diffusion path lengths through grain surfaces or along edges (which is of considerable interest in the analysis of atmospheric contamination and in certain radiation damage problems), and the connectivity of phases in polyphase microstructures. Three-dimensional analysis can be performed on computer simulated microstructures, [1] using "serial section" techniques of the sort employed in the experimental study of real microstructures. However, since many sections must be analyzed and correlated to obtain reasonably complete three-dimensional data, this approach is expensive in computing time if simulated and painstakingly time consuming if done experimentally.

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If we restrict attention to microstructures of the "cellular" type, that is, microstructures obtained through isotropic growth from a distribution of nuclei which form simultaneously, it is possible to construct an efficient code which will completely analyze the microstructure in three dimensions. The code is based on the geometric simplicity of cellular microstructures. Such a microstructure is completely described by a list of the nucleation sites. Grain corners are then points which are equidistant from four adjacent nucleation sites which are the nearest sites to the corner point. Grain edges are straight lines which connect corners, and contain points which are equidistant from the three nearest nucleation sites and bounded by corners. Grain surfaces are planes, equidistant from two nucleation sites, which are bounded by edges. For the purposes of computer analysis the cellular microstructure is best represented by a stored graph in which nodes represent grain corners in the microstructure and each node is connected to four other nodes by paths representing grain edges. All interesting three-dimensional geometric information can be extracted from this graph.

We have constructed an efficient computer code for creating and storing the connected graph described. Efficient searching and storing algorithms enable our code to create a connected graph for a periodic cube possessing up to three thousand nucleation sites in reasonable computation time. Figures 1 and 2 show the distribution functions for the number of faces (i.e., number of neighbors) per cell and the edge length, respectively, for a cellular microstructure containing 300 nucleation sites. Distributions for cell volumes and surface areas can also be calculated. Furthermore, linear programming techniques can be used to find the shortest edge path

through the resulting cellular microstructure. Thus, the simulation of a three-dimensional cellular microstructure should enable study of a variety of interesting problems.

REFERENCES

1. K. W. Mahin, K. Hanson, and J. W. Morris, Jr., "The Computer Simulation of Homogeneous Nucleation and Growth Processes," Conf. on Computer Simulation for Materials Application, NBS, Gaithersburg, Md. April 19-21, 1976.

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Fig. 1. The distribution of the number of faces per grain in a cellular microstructure obtained by isotropic growth from randomly distributed nucleation sites.

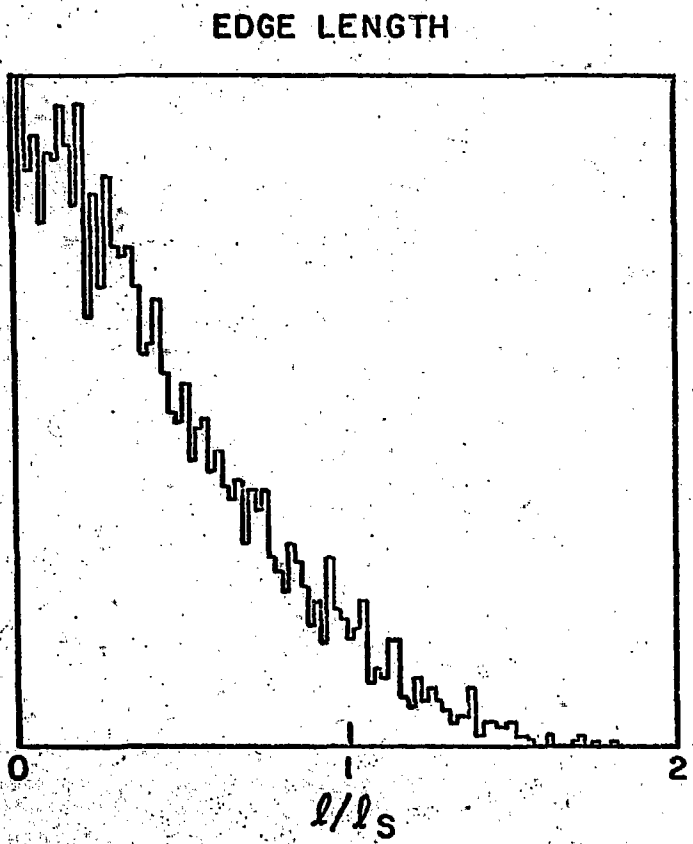

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Fig. 2. The distribution of cell edge lengths within a cellular microstructure.