MODELING GRAIN GROWTH BY THE MONTE CARLO METHOD ON ISOTROPIC GRIDS


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Results of modeling grain growth by the Monte Carlo method on grids consisting of Voronoi polyhedra for an isotropic distribution of the points on a plane and in space are reported. The influence of the grid structure on the properties of the model are discussed.

Introduction. The structure of the grains in polycrystalline materials determines, to a considerable degree, their physical properties. Considering the practical importance of these materials, it is natural that a large number of experimental works are devoted to investigation of the processes of recrystallization, grain growth, and migration of intergrain boundaries [1, 2]. Prediction and control of the grain structure encounter difficulties due to the complicated interactions and nonequilibrium processes occurring in these materials in industrial treatment. For just this reason no complete theoretical generalization of experimental data is available. Mathematical modeling of the processes of recrystallization and growth of grains is one of the possible ways of predicting the structure and properties of polycrystalline materials. Use of the Potts model and the Monte Carlo method to model the evolution of the structure of grains makes it possible to obtain the main relations and the statistical distributions typical for experimental data. Owing to this and to the simplicity of the model this approach is currently widely used.

2. Statement of the Problem. In modeling by the Monte Carlo method a material is represented as a regular hexagonal or tetragonal grid in the two-dimensional case and as a simple cubic grid in the three-dimensional case. Each \( i \)-th \((i = 0, \ldots, N)\) cell of the grid is assigned a definite "orientation" \( s_i \), and connected regions of the grid consisting of cells with the same orientation form a grain. The number of possible orientations \( Q \) is limited \((s = 1, \ldots, Q)\). The Hamiltonian of the system is written as the sum of the interaction energies of neighboring cells of the grid, and the interaction energy differs from zero only for cells with different orientations:

\[
H = -J \sum_{i,j} (\delta_{s_i s_j} - 1),
\]

where \( J \) is a positive constant; \( j \) takes the values of the original numbers of the cells adjacent to the \( i \)-th cell. For this Hamiltonian all the excess energy is concentrated at the intergrain boundaries. Simulation of migration of grain boundaries using the Monte Carlo method [3] consists for this model in modeling the process of relaxation of the system to the equilibrium state at a certain temperature \( T \) and involves the following operations: step-by-step generation of a random change in the orientation associated with thermodynamic fluctuations for a randomly chosen grid cell; conservation of the change with a probability \( \sim \exp (-\Delta E / T) \), where \( \Delta E \) is the energy increment of the system associated with the change in the orientation. In the modeling, the time \( t \) is measured in Monte Carlo steps, and each such step is equal to \( N \) attempts to change the orientation in the system.

The grids used in the modeling contain, as a rule, about \( 10^4 - 10^5 \) cells for two-dimensional models and \( 10^6 \) cells for three-dimensional models. Periodic boundary conditions are imposed to the system. Despite the simplicity, the models presented demonstrate behavior similar to grain growth in polycrystalline materials [4, 5], and introduction of additional terms into the Hamiltonian and of "special" fixed orientations makes it possible to model recrystallization [6, 7] and to take into account the influence of a second phase [8].

Although numerous works are devoted to investigation of grain growth on regular discrete grids, the influence of the grid structure has been paid little attention, and it mainly concerns the mechanisms of state transfer responsible for migration of the boundary as a whole. At the same time the influence of anisotropy and possible irregularities in the grid have not been considered. The importance of this problem is easy to understand by comparing the results of modeling on hexagonal and tetragonal grids since in these cases the evolution of the microstructure of the material is essentially different.

Below, consideration is given to grain growth on isotropic grids that are Voronoi diagrams Vor(Ω) for nodes arranged in a random manner. Construction of such a grid consists of the following steps: generation of a set of nodes \( P = \{p_1, p_2, \ldots, p_N\} \) randomly arranged inside some region \( \Omega \) \( \forall i = 1, N \); construction of the Voronoi diagram

\[
\text{Vor} (\Omega) = \bigcup_{i=1}^{N} M_i ,
\]

where \( M_i(F, V, E) \) is the Voronoi polyhedron (VP) of the point \( p_i \) determined by the set of faces \( F \), vertices \( V \), and edges \( E \):

\[
M_i = \{x| x \in \Omega, d(x, p_i) \leq d(x, p_j) \forall j \neq i \},
\]

where \( d \) is the distance between the points.

In the case of regular arrangement of the nodes of the set \( P \) according to a triangular or square template, the corresponding Voronoi diagrams form regular hexagonal and tetragonal grids on a plane; similarly, arrangement of nodes according to a cubic template leads to construction of a cubic grid in space. Thus, Voronoi diagrams are a natural generalization of the investigated cases of regular grids for sets of arbitrarily arranged nodes. In arranging nodes that prescribe a grid in a random manner, the influence of anisotropy on grain growth is excluded, and the diagrams obtained are nondegenerate. Here the order of the junctions does not exceed four in three-dimensional space and three on a plane. Properties of these diagrams and algorithms for their construction are given in [9, 10].

Modeling of grain growth in the two-dimensional case was carried out on a grid consisting of \( N = 60,000 \) randomly arranged nodes. The region \( \Omega \subset \mathbb{R}^2 \) was a unit square. For modeling of grain growth in the three-dimensional case, use was made of a grid consisting of \( N = 10^5 \) polyhedra, and the region \( \Omega \subset \mathbb{R}^3 \) was a unit cube. In all cases periodic boundary conditions were imposed on the region.

For the case of irregular grids, instead of (1) we introduce a Hamiltonian of the form

\[
H = -J \sum_{i,j} S_{ij} (\delta_{s_i, s_j} - 1) ,
\]

where \( S_{ij} \) is the area of the face of the \( i \)-th polyhedron in common with the \( j \)-th polyhedron in the three-dimensional case. In the two-dimensional case \( S_{ij} \) is the length of the corresponding edge. In (4) the energy of the system is proportional to the surface area of the intergrain boundaries, and modeling by the Monte Carlo method leads to minimization of the surface energy of the grains.

Complication of the form of the Hamiltonian and the structure of the initial discrete grid increases considerably the computational expenditures and the requirements on the size of the memory in modeling. Difficulties are encountered, foremost, in construction of large grids, and therefore effective parallel algorithms [10, 11] for