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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:

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

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 ΔE 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].

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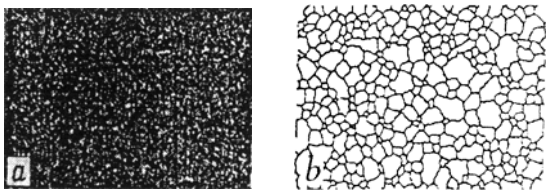

Fig. 1. Structure of grains at the initial moment of time $t = 0$ (a) and $t = 10^5$ μsec (b) at $T = 0.5T_c$.

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 Ω ($p_i \in \Omega$, $\forall i = 1, N$); construction of the Voronoi diagram

$$\text{Vor}(\Omega) = \bigcup_{i=1}^{N} M_i, \tag{2}$$

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:

$$M_i = \left\{x \mid x \in \Omega, d(x, p_i) \leq d(x, p_j) \ \forall j \neq i\right\}, \tag{3}$$

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 $\Omega \subset R^2$ 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 $\Omega \subset R^3$ 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

$$H = -J \sum_{i,j} S_{ij} (\delta_{s_i, s_j} - 1), \tag{4}$$

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

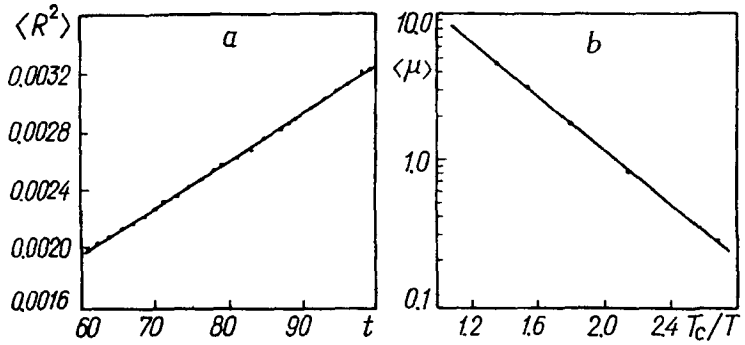

Fig. 2. Mean grain area versus time at $T = 0.7T_c$ (a) and mean mobility of grain boundaries versus temperature (b).

construction of two- and three-dimensional Voronoi and Delone diagrams were developed for the parallel computation system PowerXplorer of the Parsytec firm. To decrease computational expenditures in grain growth modeling, corresponding parallel algorithms and an algorithm for balancing the loading of the processors based on modeled annealing (a problem of discrete mathematics) were also developed [11].

The number of possible orientations Q was varied from 2 to N in the calculations. With increasing Q the volume of calculations increases proportionally. It was established numerically that the influence of coalescence of grains with the same orientation on the system properties becomes negligible for $Q \sim 100$. In all cases a random distribution of orientations over the grid cells was adopted as the initial distribution. To obtain reliable results for the self-similar regime of growth, statistical distributions and relations of the growth parameters were determined starting from the moment when approximately 500 grains remained in the system, and the mean grain contained $\sim 10^2$ cells of the initial grid. As a whole, the results of modeling on the two-dimensional and three-dimensional models showed the same behavior of the systems at large times; however the accuracy of the results in the two-dimensional case was higher.

2. Results of Modeling. In all the cases under consideration the modeling showed absence of grain growth at $T = 0$. However, at $T > 0$ stable normal growth was observed at large times of $\sim 10^5$ μsec (Monte Carlo steps). Measurements were made in the temperature range of $(0.3-0.8)T_c$. In the modeling, the area and topological class of each grain were determined every few steps of the Monte Carlo method. A typical pattern of the grain structure is shown in Fig. 1, where mainly triple junctions in the system are seen to approach equilibrium, as has been observed in experiments [1, 12].

In the modeling, a linear law of growth of the mean grain area $\langle R^2 \rangle \sim t$ was obtained for the entire temperature range. Correspondingly, for the mean grain radius the relation $\langle R \rangle \sim t^n$, where $n \approx 0.50 \pm 0.03$, is obtained. The dependence of the mean grain area on the time for $T = 0.7T_c$ is shown in Fig. 2a. Unlike the results of modeling on regular grids, in the cases under consideration the actual area of the grains was calculated instead of the number of cells of the initial grid in a grain, since the sizes of the cells are not equal. For the initial stage of grain growth the exponent gradually increases starting from $n \approx 0.26$.

The distribution of the grains over the areas and the topological classes turned out to be invariant in time. As is seen in Fig. 3, the distributions correspond to normal grain growth and are close to those observed experimentally for pure metals [12].

The mobility of the grain boundaries μ [1] obeys, as the modeling showed, an Arrhenius law with a constant activation energy W in the investigated temperature interval:

$$\langle \mu \rangle = A \exp(-W/T). \tag{5}$$

The mean mobility versus the temperature is shown in Fig. 2b. At the same time on small scales strong nonuniformity of the motion of some segments of boundaries caused by the inhomogeneity of the grid, namely, different sizes and an irregular form of some cells of the initial grid, was observed. For this reason cells of large sizes hindered the motion of boundaries on some segments, thus making it stepwise. Such motion of boundaries was also observed in some physical experiments [1].

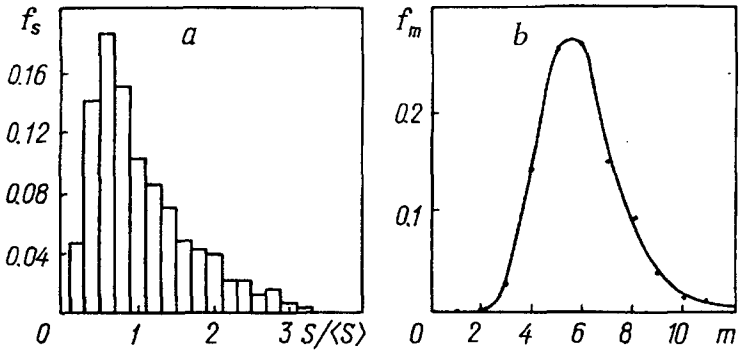

Fig. 3. Distribution of grains over areas (a) and topological clsasses (b).

To study the influence of the structure of the initial discrete grid on the grain-growth parameters, we investigated the behavior of the model in the case of step-by-step recovery of the symmetry from the Voronoi diagram for an isotropic distribution of the nodes up to a regular hexagonal grid in the two-dimensional case. At each step of the recovery of the ordering each point of the set P moved due to the effective repulsive force acting from the side of the nearest neighbors. As a result, the symmetry appeared in the grid after a certain time. Investigation of the model parameters at each step showed that in this recovery the activation energy of the system decreases rapidly, while the index n of the degree of grain growth is characterized by a gradual increase in value at small times up to 0.4 and an increase in the transient period.

Conclusion. Numerical investigations performed on models with regular and irregular grids demonstrate many universal properties and relations typical for grain growth in polycrystalline materials. Here the choice of the initial discrete grid exerts a considerable influence, as calculations showed, on the behavior of the model and opens possibilites for more adequate matching of the grid structure with the structure of a real polycrystal.

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NOTATION

N, number of cells in the grid; H, Hamiltonian of the system; J, energy of interaction of neighboring cells per unit area; δ_{ij}, Kronecker symbol; P, probability of a change in orientation; T_c, critical temperature; R, grain size; n, index of the degree of grain growth; A, preexponential factor; f_S, f_m, distribution functions over areas and topological classes; S, grain area; m, topological class of a grain. All quantities are dimensionless.

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