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RECRYSTALLIZATION STUDY USING TWO-DIMENSIONAL VERTEX MODEL

BADANIE REKRYSTALIZACJI PRZY UŻYCIU DWUWYMIAROWEGO MODELU TYPU VERTEX

Recrystallization process in polycrystalline material was studied using two–dimensional model based on vertex concept. Initial microstructure is characterized by topology, crystallographic orientations and stored energy values of grains. The boundary energies and mobilities are anisotropic in general. Additional forces, being driving ones in recrystallization, are exerted on vertices and they are derived from the stored energy gradients between adjacent grains. Nucleation mechanism of a given type is selected at the beginning of calculations. Two types of nucleation were tested. Deformation texture, stored energy distribution and initial microstructure are input parameters of the model. They were obtained from X-ray and EBSD measurements. The goal of the calculations is the prediction of texture and microstructure modification during recrystallization. Comparison of predicted and experimental characteristics enables verification of model assumptions. par *Keywords*: Recrystallization, vertex model, triple point, grain boundary energy, stored energy, nucleation, crystallographic texture

Przeprowadzono badanie procesu rekrystalizacji materiału polikrystalicznego przy użyciu dwuwymiarowego modelu typu „vertex". Początkowa mikrostruktura materiału opisana jest przez topologię, orientację krystalograficzną oraz energię zgromadzoną ziaren. Energia granic i ich ruchliwość są na ogół anizotropowe. Dodatkowe siły, działające na węzły, pochodzą od gradientu energii zgromadzonej w sąsiednich ziarnach; są one siłami napędowym rekrystalizacji. Mechanizm zarodkowania ustalany jest na początku obliczeń. Przetestowano dwa typy zarodkowania. Tekstura deformacji, rozkład energii zgromadzonej oraz początkowa mikrostruktura są parametrami wejściowymi modelu. Uzyskano je techniką dyfrakcji rentgenowskiej oraz techniką dyfrakcji elektronów rozproszonych wstecznie. Celem obliczeń jest przewidywanie zmian tekstury oraz mikrostruktury podczas rekrystalizacji. Porównanie charakterystyk obliczonych ze zmierzonymi pozwala na weryfikację przyjętych w modelu założeń.

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1. Introduction

Recrystallization is one of the most frequent phenomena occurring in technological processes leading to modification of material properties. Several models of recrystallization are described in the literature. The most important types of them are: Monte-Carlo model [1] based on global energy minimization concept, vertex model [2, 3] considering forces acting on triple junctions between grain boundaries, cellular automata algorithm [4], compromise function concept [5, 6] or finite elements approach [7]. Each of these models has some advantages and some restrictions. The Monte-Carlo concept is very efficient and relatively easy to apply to complex microstructures. On the other hand, some problems with grain boundary curvature implementation can occur. The vertex model is based on similar assumptions on grain boundary energy and its mobility as MC one. However, contrary to MC model, the vertex model is a deterministic one and there are no problems to introduce grain boundary curvature. This model was successfully used to predict abnormal grain growth [2, 3] where boundary energy and boundary types play the most important role, but till now the stored energy was not implemented in the model. Consequently, to improve the vertex model and make it more flexible, the stored energy was introduced in it. As a consequence, the full recrystallization process may be simulated in one pass, i.e.: primary recrystallization, grain growth and then abnormal grain growth.

2. Model description

Vertex model proposed by K a w a s a k i et al. [2] and developed by W e y g a n d [3] was used to simulate grain growth (i.e. the process occurring after primary recrystallization); the considered grain boundaries (GB) movement leads to the minimization of total surface energy of grains. In K a w a s a k i ' s 2D model, the evolution of grains microstructure is simulated by the movement of triple points — so called "real vertices" (triple point is a point where three GBs meet). The equations of triple point movement are derived from variational approach. Grain boundaries energies and mobilities were in both models anisotropic — they depended on crystallographic misorientation between adjacent grains. The modification introduced in the present model, based on W e y g a n d work [3], is the introduction of the stored energy, playing an important role during recrystallization. In the model presented below the microstructure of polycrystalline material is represented by two-dimensional network of vertices with positions $\vec{r}_k$, where $k = 1, \ldots N$ (N is number of vertices in structure). Each (sub)grain has a given orientation O_i and stored energy value H_i. General equation for the motion of vertices, which incorporates the orientation dependence of boundary energy and mobility, is given by (c. f. [3]):

$$D_i\vec{v}_i = \vec{f}_i - \frac{1}{2}\sum_{j}^{(i)} D_{ij}\vec{v}_j \; i = 1, ..., N, \tag{1}$$

where v_i is the *i-th* vertex velocity and j index is running over all vertices which are connected to the *i-th* vertex. D_{ij}, D_j and $\vec{f_i}$ are given by (c. f. [3]):

$$D_{ij} = \frac{1}{3m_{ij}\left\|\vec{r}_{ij}\right\|}\begin{pmatrix} y_{ij}^2 & -x_{ij}y_{ij} \\ -x_{ij}y_{ij} & x_{ij}^2 \end{pmatrix} \tag{2}$$

$$D_i = \sum_j^{(i)} D_{ij} \tag{3}$$

$$\vec{f_i} = -\sum_j^{(i)} \sigma_{ij}\frac{\vec{r}_{ij}}{\left\|\vec{r}_{ij}\right\|} + \sum_j^{(i)} \gamma_{ij}\vec{n}_{ij}. \tag{4}$$

In the above equations m_{ij} is the mobility of grain boundary between vertices i and j, the vector $\vec{r}_{ij} = \begin{pmatrix} x_{ij} \\ y_{ij} \end{pmatrix}$ is defined as $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$ (where $\vec{r}_i$ and $\vec{r}_j$ are positions of i-th and j-th vertex) and σ_{ij} is the grain boundary energy between vertices i and j. In Eq. 4 the term γ_{ij} was added, which describes the stored energy gradient. It is approximated by: $\gamma_{ij} = H - H'$, where H and H' are values of stored energy in grains adjacent to segment (edge) between vertices i and j. Unit vector $\vec{n}_{ij}$ is perpendicular to the vector $\vec{r}_{ij}$.

Values of mobility m_{ij} and grain boundary energy σ_{ij} depend on misorientation angle ϕ between two adjacent crystallographic lattices. For low angle grain boundaries ($\phi < \phi_m \approx 15°$), the Read-Shockley relation is applied:

$$\sigma(\phi) = \sigma_{HAGB}\frac{\phi}{\phi_m}\left(1 - \ln\frac{\phi}{\phi_m}\right), \tag{5}$$

where σ_{HAGB} is a high angle grain boundary energy. Dependence of mobility m on misorientation angle ϕ is given by [8]:

$$m(\phi, B, n) = m_{HAGB}\left(1 - \exp[-B(\phi/\phi_m)^n]\right), \tag{6}$$

where m_{HAGB} is mobility of high angle grain boundary, B and n are constants. Values of m_{HAGB} for boundaries between two deformed grains (with high values of stored energies) are lower then for boundaries deformed grains and nuclei. Velocities of vertices are calculated from Eq. (1) in each model iteration. Once the velocities of vertices at time t are already known then the maximal possible time step is calculated. The time step dt is chosen so that any segments (edge) should not change its length more than a fraction $f = 0.5$. The new positions of vertices are given by:

$$\vec{r}_i(t + dt) = \vec{r}_i(t) + \vec{v}_i(t) * dt. \tag{7}$$

The initial positions of vertices in the grains are the corners of a Voronoi structure. At the very beginning of simulation new nuclei are placed in chosen grains. Site

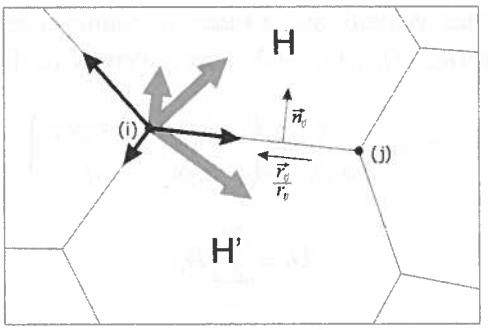

Fig. 1. Forces exerted on the i-th vertex; forces derived from surface tension are marked with black solid line while those derived from the stored energy gradient — with gray

saturated nucleation was implemented in the model — nuclei are placed in grains before they start to grow. Stored energy value H inside each nucleus is set to zero. Two different types of nucleation were used and tested in the model: *random nucleation* — nuclei are distributed in randomly chosen grains, and *preferred nucleation* in which the probability of placing nucleus inside a randomly chosen grain is proportional to its stored energy value H. Orientation of a new nucleus is derived from an original grain and its stored energy value is set to zero. The example of a grain with a new nucleus placed inside is presented in Fig. 2. To fulfill the requirements concerning triple points the additional edges are introduced.

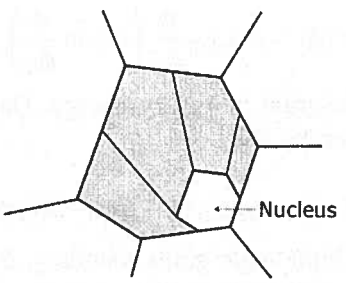

Fig. 2. Placing a new nucleus into the structure

During recrystallization process, the grain structure undergoes topological changes. Besides two well known topological transformations — the recombination of triple points (T1 process) and shrinking of triangular grain (T2 process) — a new transformation (named TA) had to be introduced. The latter transformation is necessary when one of the vertices is approaching a grain edge (edge BC on Fig. 3c); it appears only if the stored energy gradient between grains is introduced. Minimal distance Δ, allowed between adjacent vertices, is proportional to $<r>$ — average radius of the grains.

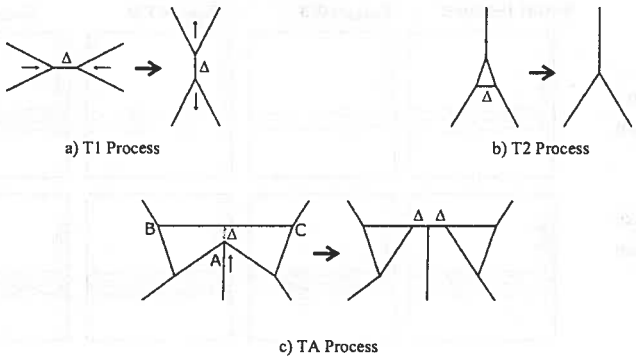

Fig. 3. Topological transformations of the simulated grain structure used in the model

3. Recrystallization of low carbon steel

A model texture (of cold rolled low carbon steel), composed of 8 ideal components, used by W i m m e r [9], was applied (Table 1). Two types of nucleation were tested in

TABLE 1

Ideal components of the model cold rolling steel texture, their participations and used stored energy values; α and γ are two main fibers of this texture (ϕ_1, Φ, ϕ_2 are Euler angles)

Fiber	ϕ_1	Φ	ϕ_2	Particip. (%)	Stored energy (relative units)
α	45	90	0	7.25	3.0
	0	19	45	10.25	3.5
	0	25	45	15.25	3.5
	0	35	45	20.25	4.0
γ	19	54	45	11.25	6.0
	10	54	45	11.25	6.0
	90	54	45	12.25	6.0
	0	54	45	12.25	6.0

the model: random and preferred one. In the latter case, nuclei appear preferentially in the high stored energy regions (with probability proportional to H). On the other hand, different values of high angle grain boundary energy were used (E_{HAGB} = 0.3, 1 and 3 — in relative units). The results of texture prediction are shown in Fig.5 (ODF section for $\phi_2 = 45°$ are shown). We find that preferred nucleation predicts more correct texture change then random nucleation, i.e., the strengthening of γ fiber (the horizontal one), and gives the textures more similar to these commonly experimentally observed [10]. We also find that, with increasing E value, the γ fiber is much reinforced, even with random nucleation. In conclusion, the preferred nucleation and high grain boundary energy lead to the correct predictions of texture change during recrystallization.

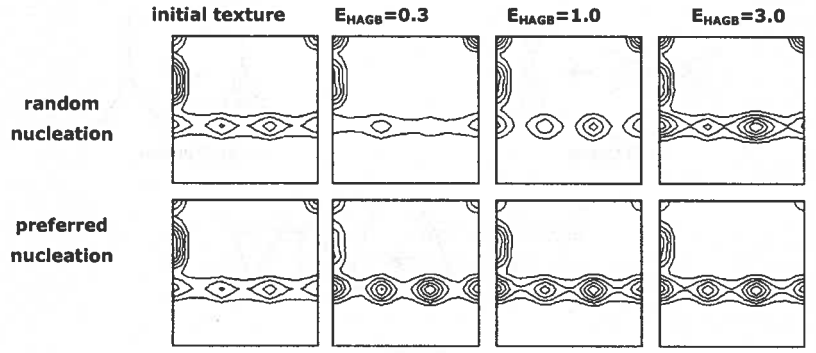

Fig. 4. Predicted texture changes during recrystallization of the model cold rolling steel texture ("initial texture"). Three values of the grain boundary energy were used (E=0.3, 1 and 3); random and preferred nucleation was considered

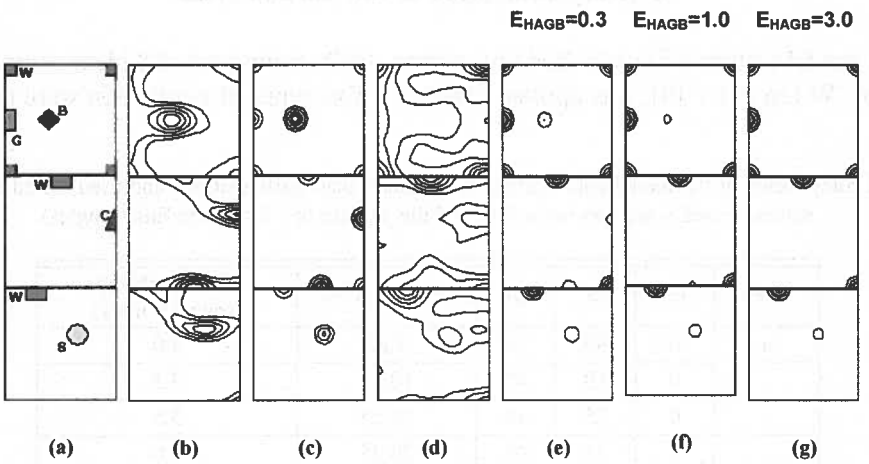

Fig. 5. Predicted texture changes during recrystallization of the polycrystalline copper: (a) ideal components, (b) deformation texture, (c) discretized deformation texture, (d) predicted recrystallization textures for different grain boundary energies (e,f,g)

4. Recrystallization of copper

Deformation texture of copper was discretized into 5 ideal orientations. Values of stored energy for ideal orientations were measured using XRD technique by G e r b e r et al. [12]. Set of initial orientations and stored energy values used as input data for modelling is presented in Table 2.

Calculations for copper were performed without nucleation and for three different values of high angle grain boundary energy — E_{HAGB} (similarly like in the case of steel). Predicted final textures of recrystallization and their comparison with experimental one are presented in Fig.6. Simulated recrystallization textures show similarity to experimental ones. Reinforcement of cubic orientation (W) and weakening of copper

TABLE 2
Ideal components of the model cold rolling copper texture, their participations and stored energy values (estimated from XRD measurements)

Ideal orientation	ϕ_1	Φ	ϕ_2	Particip. (%)	Stored energy (relative units)
W	0	0	0	7	1.05
B	35	45	0	27	5.70
C	90	35	45	26	6.00
S	59	37	63	32	4.65
G	0	45	0	8	1.35

(C), brass (B) and S orientations are in agreement with experimental observations. On the other hand, Goss (G) orientation remains too strong in modeled textures. This suggests an occurrence of another mechanisms during recrystallization, which was not considered in the model.

5. Conclusions

Two dimensional vertex model was generalized by the introduction of stored energy distribution. Both random and preferred nucleation was examined. The influence of grain boundary energy was also studied. The present vertex model was tested on the textures of cold rolled low carbon steel and of polycrystalline copper, deformed to 70% rolling reduction; these textures were discretized into some number of ideal orientations. In the case of low carbon steel, the correct predictions of texture change were obtained for higher grain boundary values and for the preferred nucleation (with nucleation probability proportional to the stored energy). For polycrystalline copper, the simulations were performed without nucleation. Predicted recrystallization textures exhibit strong similarities to experimental ones. However, some small discrepancies show that another phenomena, appearing during recrystallization, should be also taken into account in the modelling.

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REFERENCES

[1] D. J. Srolovitz, G.S. Grest, M.P. Anderson, Acta Metall. **34**, 1833 (1986).
[2] K. Kawasaki, T. Nagai, K. Nakashima, Phil. Mag. B, **60**, 399 (1989).
[3] D. Weygand, Y. Brechet, J. Lepinoux, Phil. Mag. B, **78**, 329 (1998).
[4] J. Kroc, V. Paidar, Proc. of the First Joint Intern. Conf. REX & GG (eds. G. Gottstein and A. Molodov) **1**, 245 (Springer-Verlag, Berlin 2001).

[5] K. Sztwiertnia, Arch. of Metall. **41**, 101-116 (1996).
[6] K. Wierzbanowski, J. Tarasiuk, B. Bacroix, K. Sztwiertnia, P. Gerber, Metals and Materials Int. **9**, 9-14 (2003).
[7] M.C. Demirel, A.P. Kuprat, D.C. George, B.S. El-Dasher, G.K. Straub, A.D. Rollet, Proc. of the First Joint Intern. Conf. REX & GG (eds G. Gottstein and A. Molodov), P**1**, 297 (Springer-Verlag, Berlin 2001).
[8] F.J. Humphreys, M. Hatherly, Recrystallization and Related Annealing Phenomena, (Pergamon Press, Oxford 1995).
[9] M. Wimmer, M. Kiaei, B. Bacroix, S. Lanteri, H. Reglé, IRSID Report no. MPM 96.769 (IRSID, Maiziers-les-Metz, France 1996).
[10] K. Wierzbanowski, J. Tarasiuk, B. Bacroix, A. Miroux, O. Castelnau, Arch. of Metall. **44**, 183-201 (1999).
[11] K. Piekos, J. Tarasiuk, K. Wierzbanowski, B. Bacroix, Development of Two — Dimensional Vertex Type Model, Materials Science Forum **467-470**, 653-658 (2004).
[12] Ph. Gerber, J. Tarasiuk, B. Bacroix, Mat. Sc. Forum **408-412**, 851 (2002).

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