DIFFUSIONAL RECONSTRUCTION OF LOW-ANGLE TILT GRAIN BOUNDARY IN ORDERED ALLOY CUAU

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The article deals with the results of a computer study of random tilt grain boundaries (GB) in Al. GB's axis of turn is [100] with misorientation angle of 9^0. The atomic interaction was approximated by Morse's semi-empirical potential. Minimisation of a defect crystal energy was carried out by using vacancy and shift relaxation. Vacancy relaxation was achieved by removing atoms from the defect area. Shift relaxation was analysed by constructing γ-surface. It has been shown that GB has a stable and a metastable states. Transition from one state to the other takes place as a result of diffusion processes. Transition to a metastable state makes displacement of one grain relatively the other easier and reduces stress of GB sliding.

1. Introduction

A theoretical research of low-angle GB's structure and energy in the majority of works has been carried out using dislocation model [1]. This model is based on continuity theory of elasticity, it does not take into account GB's discrete atomic character and does not allow to reveal many details of the thin GB structure. Studying the thin structure is necessary for understanding elementary acts of GB rearrangement such as GB sliding. Micromechanisms of GB sliding have not been investigated so far. It has been proved by experiments that GB sliding is activated under the influence of diffusion processes [2]. Computer simulation is an effective method of such studies. For this study calculation of GB energy and structure has been done in a semi-rigid model in which atoms remain in the lattice sites of corresponding grains. Atom diffusion has been investigated only in GB core.

2. Theory

Energy Calculation

A thin GB structure study has been carried out for low-angle symmetrical tilt GB 9^0 [100] in Al. Such GB may be formation at misorientation on angle 9^0 by a turn around axis [100]. For this misorientation angle the boundary has a non-periodical structure. Atomic interaction was approximated by Morse's empirical potential. Parameters of the potential and the procedure of it receiving are described in [3]. Defect energy was defined as the difference between an ideal crystal and a defect crystal energies. For energy calculation atom interaction in four coordinate spheres was taken into account.

Axis of turn [100] was chosen in such a way that after defect formation it crossed coincidence sites of two misorientated lattices. The coincidence site is the starting point of calculation. In Fig.1a GB structure projected to plane (100) is shown. The coincidence site is marked with the letter "O". OY axis is parallel to the axis of turn, OX axis is parallel to the GB plane, OZ is normal to the GB plane. GB has the identity period along to OY of a=0.478 nm (a - the lattice constant). There is no identity period along to OX axis. The value of calculated area along an axes OX was equal

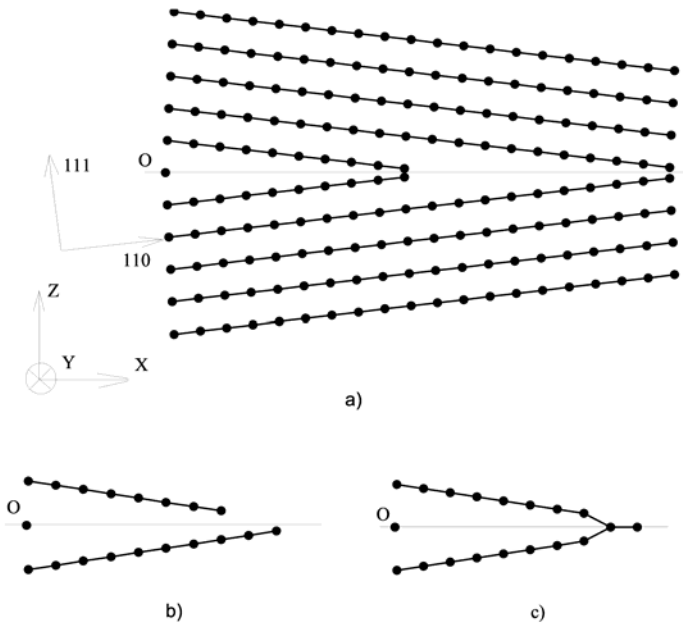

Fig. 1. GB structure projected to plane (112): a - non-relaxed;
b - GB with a localised vacancy;
c - GB with a distributed vacancy. O - coincidence site

16.31a=6.493 nm. Local energy E_x was calculated for the accounted cell having a square in GB plane falling at one atom. Average energy E was defined taking into account the whole area of calculated GB.

At the formation of GB some of the atoms converge. Atom convergence increases the defect energy sharply. Such a boundary is energetically inefficient and must relax. Two variants of relaxation were investigated: (1) relaxation with the change of atom quantity per a GB (vacancy relaxation) and (2) relaxation with additional shift (shift relaxation).

Vacancy Relaxation

Vacancy relaxation was carried out in two ways: by introducing into the boundary core (1)localised and (2)distributed vacancies [4]. The structure of GB core and the variants of relaxation are shown in Fig.1. The procedure of vacancy introduction was accomplished in the following way: couples of atoms converged to a distance less than r_{min} were determined. One of such atoms was moved from GB core on a surface of crystal. A localised vacancy appeared in its place. Calculation of GB with a localised vacancy energy E_l was made. After that the remaining atom was moved to the GB plane and energy E_d of GB with a distributed vacancy was calculated.

Fig.2 shows the distribution of GB local energy E_X along OX axis. Each curve corresponds to one step of relaxation procedure. Curve 1 shows the energy distribution after the removal of atoms the distance between which was $r_{min}<0.5r_1$ (r_1 - radius of the 1st coordination sphere). The peaks of energy correspond to the areas of GBs with strong convergence of atoms. Curves 2, 3, 4 were received after repeated procedure of atom removal. Curve 5 shows the energy of a completely relaxed boundary. GB's average energy was calculated at each stage of relaxation procedure. GB's average energy changes in the process of step-by-step relaxation are shown in Fig.3. Curve 1 shows this dependence for a defect with localised vacancies, curve 2 - with distributed vacancies. Minimal values E_l^s and E_d^s may be considered as defect energy and correspond to stable states of GB. In Fig.3

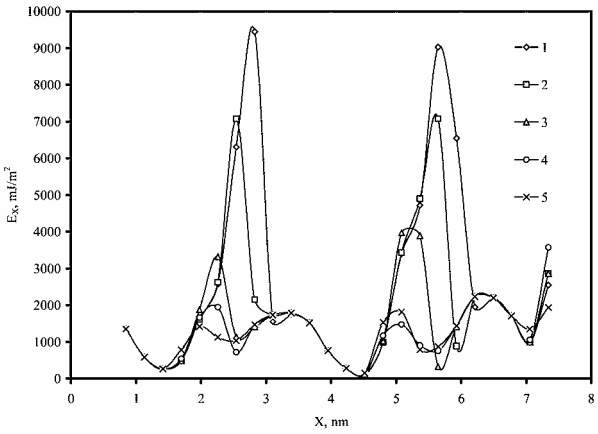

Fig. 2. Local energy E_X distribution along the GB length. Curve number (1-5) shows the stage of relaxation

stable states are marked as s^l and s^d for GBs with localised and distributed vacancies respectively. A change in atom concentration per a GB increases the energy and converts the defect into a metastable state. The state of a GB with atom excess is marked as m_1, with

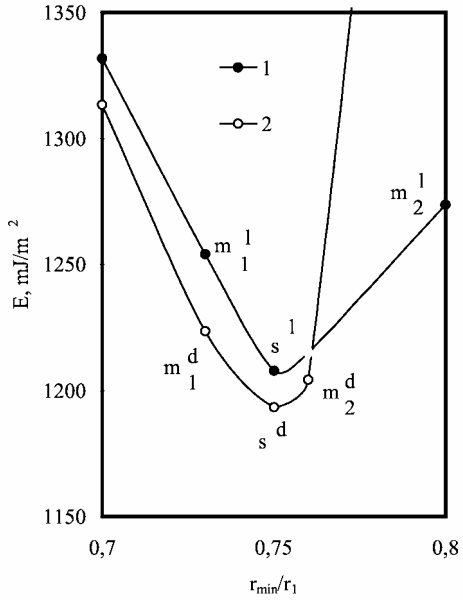

Fig. 3. Change of GB average energy at removal from the core one of the two atoms, the distance between which is less than r_{min}; 1 - GB with localised vacancies; 2 - GB with distributed vacancies. s-stable states, m_1 end m_2 - metastable states with atom and vacancy excess respectively. Indexes l and d refer to GBs with localised and distributed vacancies. r_1 - radius of the 1st coordination sphere

vacancy excess - m_2 (Fig.3), respective energies are listed in table 1.

Table 1

GB energy (mJ/m^2) after carrying out vacancy and displacement relaxation. s - stable state, m_1 and m_2 - metastable states with atom and vacancy excess respectively

State	Vacancy relaxation		Shift relaxation (**f** state)	
of GB	Localised	distributed	localised	distributed
m_1	1256	1224	1188	1725
s	1208	1193	1243	1340
m_2	1274	1204	1168	1418

Shift Relaxation

A GB shift relaxation study was carried out by γ-surface construction [5]. A rigid model was used for γ-surface calculation. One grain was displacement relatively the other on vector **R**. With displacement the atoms remained in the sites of corresponding lattices. After each displacement by 0.024 nm average energy E was calculated. The calculations were made for stable (s) and metastable (m_1, m_2) GB states.

The γ-surface for a metastable GB with localised vacancies is shown in Fig.4 as an example. Position at $\mathbf{R_X} = \mathbf{R_Y} = 0$ corresponds to GB after vacancy relaxation. At this point γ-surface has its minimum. Another important feature of γ-surface is the minimum at the displacement by a some $\mathbf{R_f}$ vector. It means that there exists a steady state **f** into which GB can transfer as a result of displacement. Energies of **f** state are shown in table I.

3. Results

GB energy calculations have shown that several steady states of defect exist. One of them is stable, others are metastable. A GB can have increased energy as a result of excess number of atoms or vacancies in a core. An atom or a vacancy removal from a GB area is necessary for transition to a metastable state. Such a rearrangement of a GB can happen is the result of diffusion.

Calculations made in this study for Al have shown that a distributed vacancy state is energetically preferable (table I). The received results are in good accordance with the data of a computer simulation of a symmetrical tilt GBs of special type Σ=7 in Au [6]. Direct investigation by high-resolution transmission-electron microscopy tilt GB Σ=5[100](013) in Al-5%Mg alloy [7] and in Au [8] also reveal that atomic structure of GB has a relaxed state of a distributed vacancy type.

After the vacancy relaxation GBs are stable in relation to displacement deformations. Their position on γ-surface corresponds to minimum. For a displacement of one grain relatively the other an external stress is necessary.

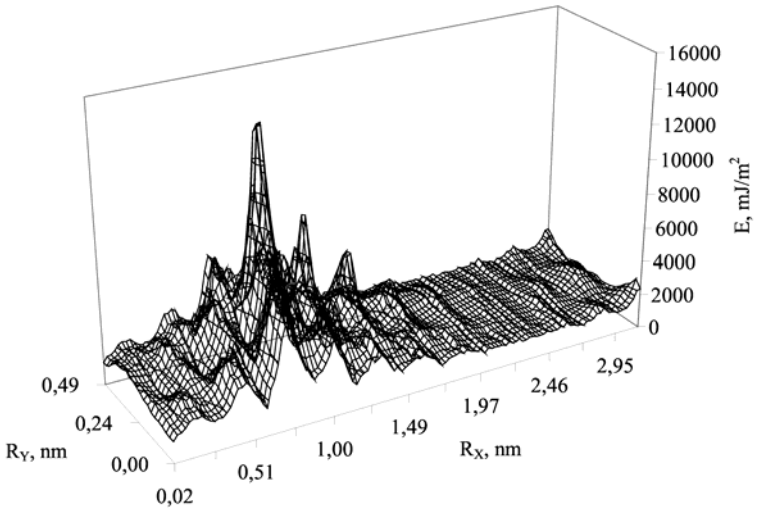

Fig. 4. General view of γ-surface of a metastable GB with localised vacancies

Existence of minima on γ-surface at some

displacement vectors $\mathbf{R} = \mathbf{R_f}$ mean the existence of intermediate steady states f. Transition from one stable state to another can take place via intermediate state f.

The results of calculation given in table I show a substantial energy increase at displacement of a GB with a distributed vacancy. In case of localised vacancies the energy either increases slightly (s^1 state) or decreases (states m_1^1 and m_2^1). For GB sliding defect rearrangement is necessary. A GB with a distributed vacancy state has minimal energy, i.e. is stable, but with an external force influence the boundary must pass into the state with a localised vacancy. As a result its energy increases only by 15 mJ/m^2. Such a change of structure allows to decrease the high potential barrier which exists at a GB with a distributed vacancy displacement.

Results of our calculations make it possible to explain activation of GB sliding processes at diffusion [2]. At raised temperatures a GB can transfer into a metastable state. Presence of atom or vacancy excess quantity per a GB (state m_1 or m_2) decreases the value of the shift deformation potential barrier and makes GB sliding easier.

4. Conclusion

Computer simulation of symmetrical low-angle tilt GB in Al have been described in the article. The calculations have shown that GB energy depends on vacancy concentration in GB core. A stable GB converts

into a metastable one both at increase and decrease of vacancy concentration. Displacement of one grain relatively the other, e.g. GB sliding is connected with potential barrier overcoming. GB transition into a metastable state can decrease the value of potential barrier and make GB sliding easier.

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