STRUCTURE AND EXESS VOLUME OF GRAIN BOUNDARIES IN METALS

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A computer simulation of symmetrical tilt GBs Σ= 5 [100] (012) in Al and Fe has been carried out. GB energy and structure were investigated by γ-surface formation. GB energy was calculated with the use of rigid and atomic relaxation. Atomic interaction was described by Morse's empirical potential. Relaxation along the perpendicular to GB plane was used to define the exess volume. Variants of GB sliding have been investigated and directions and values of potential barriers have been found. The results of the calculations are compared with the model of coincidence site lattice.

1. Introduction

Grain boundaries (GB) render large influence on many physical and mechanical properties of polycrystalline materials, as well as plastic deformation, diffusion, creep [1]. The mechanisms of the GB influence on properties of materials are now still unsufficiently investigated. It is connected with the fact that there are few data on the GB atomic structure.

The GB atomic structure is frequently investigated in a geometric model of the coincidence site lattice (CSL) [2]. However experimental researches made with the use of high-resolution transmission-electron microscopy have detected the GB properties not described by the CSL model: exess volume, relative displacements, metastable states [1, 3, 4]. Nowadays computer simulation of defects is a perspective method of defect study. The calculations of the GB structure by computer simulation methods are in good accord with experimentally observable properties [5, 6]. To receive reliable data on the structure and energetics of GB the comparison of results obtained in the CSL model and in computer simulation is necessary.

2. Theory

In the article a computer simulation of symmetrical tilt GBs in Al and Fe was carried out. Special GB Σ= 5 [100] (012) was simulated. The atomic interaction was approximated by Morse's empirical potential. Morse's potential parameters were determined using equilibrium properties of metals: lattice constant, cohesive energy, elastic constants. The radius of potentials' operation is limited by the 4-th coordination sphere. The potentials were approbated in calculation of energy and structure of vacancy, stacking faults, twins and showed a good accord with experimental data [7, 8].

The GB energy was determined as the difference between bicrystal energy, containing the boundary, and the energy of ideal crystal with identical amount of atoms. The analysis of the GB energy was carried out by the γ-surface construction method [9]. The γ-surface represents a potential relief, existing in shift of one grain relatively to the other by some vector f along the boundary plane. The research of the γ-surface allows to select a stable atomic structure of GB possessing a minimum energy. The GB [100] (012) formation in the CSL model is possible to present as a turn of one half of ideal crystal relatively to axes [100] by an angle 53.13°. As the result of this operation a bicrystal

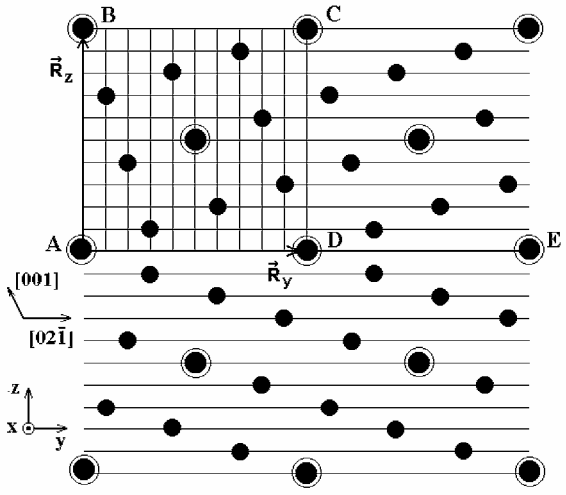

Fig.1. A structure of GB [100] (012) in Al. Two planes in a projection along the axes [100] are shown. By the large circles the coincidence sites lattice are marked. ABCD - the CSL unit cell. $\mathbf{R}_x$ and $\mathbf{R}_y$ - the basic CSL vectors. The plane of a defect - AE. In the ABCD area the DSC lattice is shown

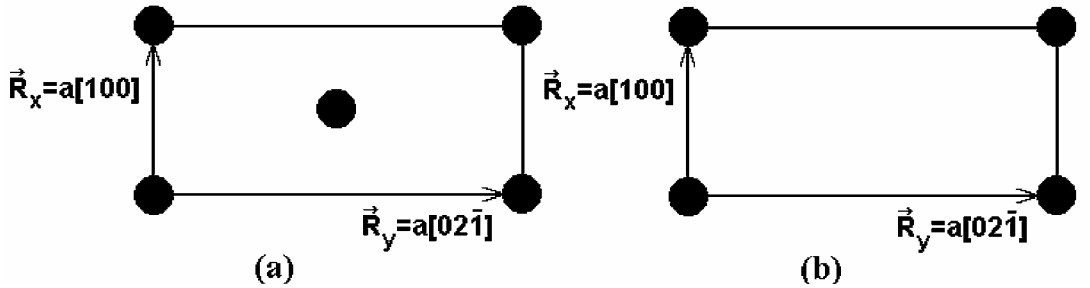

Fig.2. The unit cells in plane of GB: a - Al, b – Fe

is formed with the dividing boundary crossing the plane (012), common for both grains.

In Fig.1 the GB [100] (012) atomic structure for a fcc lattice of Al in projection to plane (100) is shown. The plane of symmetry is the GB plane. The coincidence sites are marked by circles of a large size. The unit cell of CSL has basis vectors R_X=a[100], R_Y=a[02 $\bar{1}$] and R_Z=a[012] and is marked in Fig.1 as ABCD. Inside the CSL unit cell the displacement shift complete lattice (DSC lattice) is shown. The GB construction for Fe is carried out in a similar way.

For a construction of the γ-surfaces it's enough to make a shift of one part of crystal relatively to the other within a plane unit cell. The plane unit cell or, so-called, GB structural unit in Fig.1 is shown by a segment AD. The aspect of plane unit cells for GB [100] (012) is different in Al and Fe, as the symmetry of fcc and bcc lattices is different. The structure of plane unit cells for Al and Fe is shown in Fig.2.

For calculation of the γ-surface the GB structure in the CSL model was selected as a starting structure. The GB on the γ-surface in the CSL model is equal to a shift vector f = 0. The construction of the γ-surface was carried out both in the CSL model with a rigid shift along the fault plane and with the use of two relaxation techniques: (1) rigid three-dimensional relaxation including a displacement of a grain as the whole along the X, Y, and Z-axes and (2) full atomic relaxation.

3. Results

Grain Boundary in CSL Model

The research of a potential relief at a rigid shift is of interest for comparison of computer calculations and geometric models. In geometric models the analysis of GB dislocations and GB sliding, connected with their movement, will be carried out with the use of DSC lattice [2]. It is supposed, that the GB dislocations move along a potential relief of Peierls type, which minima are in the DSC lattice sites [10]. The γ-surface calculated in the CSL models for Al, is shown in Fig.3. At the γ-surface calculations one part of bicristal was moved as a whole along the GB plane. The atoms at shifting remained in sites of corresponding lattices. The γ-surface has a complicated relief. The basic elements of the γ-surfaces are minima and maxima. The highest maxima correspond to atoms located in a GB plane. The minima determine steady states of the GB at shifting. In Fig.3b the minima are marked by shading. At f = 0 there are maxima on the γ-surface, i.e. the atomic GB structure in the CSL model is unstable. The GB stabilization can be reached by transition to the nearest minimum. The GB energy in the CSL E_{CSL} model for Al and Fe is listed in table 1.

In Fig.3b the DSC lattice, marked on the contour plot of the GB γ-surface is shown. It is visible, that the potential relief of the γ-surface does not reflect a structure of the DSC lattice. Majority of special

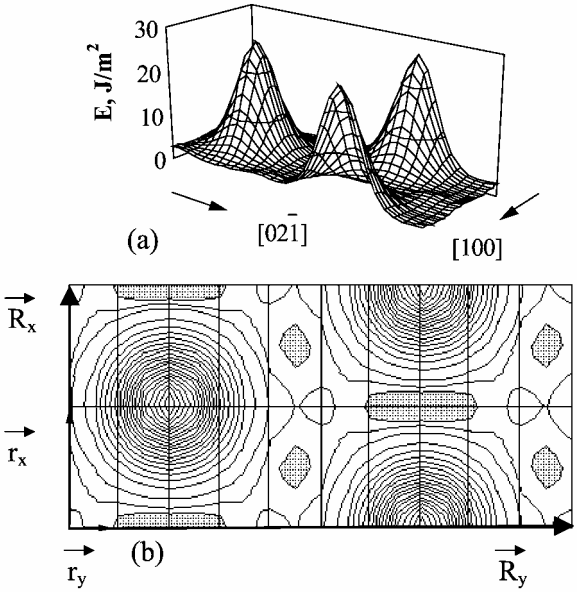

Fig.3. The γ-surface (a) and contour plot its relief (b) for the GB [100](012) in Al in the CSL model. $\mathbf{R}_x$, $\mathbf{R}_y$ are the basic vectors of the CSL unit cell, $\mathbf{r}_x$ and $\mathbf{r}_y$ - basic vectors of a unit cell of the DSC lattice. A grid - the DSC lattice in the GB plane, shaded areas - minima of energy

points of the γ-surface - minima, maxima and the saddle points do not coincide with the DSC lattice sites.

Table 1

The calculated values of the GB energy [100] (012) in Al and Fe in the CSL model - ECSL, after a rigid relaxation E_R and after an atomic relaxation E_A; shift values f and exess volume $\Delta v/v_0$

Metall	Energy, mJ/m^2			Displacement **f** , A^0			Exess volume ,
	E_{CSL}	E_R	E_A	$\mathbf{f}_x$	$\mathbf{f}_y$	$\mathbf{f}_z$	$\Delta V/ V_0$
Al	2670	1420	880	0	0	0.26	0.28
Fe	9644	1650	1088	1.43	1.55	0.026	0.04

The γ-surface of GB in Fe was also investigated and the similar conclusions were obtained. The made calculations show limited applicability of the CSL model for a research of a GB structure. It is connected with the fact that the geometric criterion of a structural stability is the basis of the CSL model whereas the energy criterion is more important.

The Relaxed Grain Boundary

The high values of GB energy in the CSL model are connected with atoms convergence at a tilt boundary forming. For determination of a stable GB structure it is necessary to make a relaxation of a crystal with a defect. The use of two relaxation techniques in the present work (rigid three-dimensional and atomic ones) allows to investigate a GB structure more completely.

The rigid three-dimensional relaxation allows to displace grains as a whole in three directions: along X, Y and Z. After realization of a rigid relaxation the GB energy E_R is essentially reduced. In table 1 the GB energy ER and the components of the displacement vector f from the CSL structure are listed. The components of a displacement vector are different for Al and Fe.

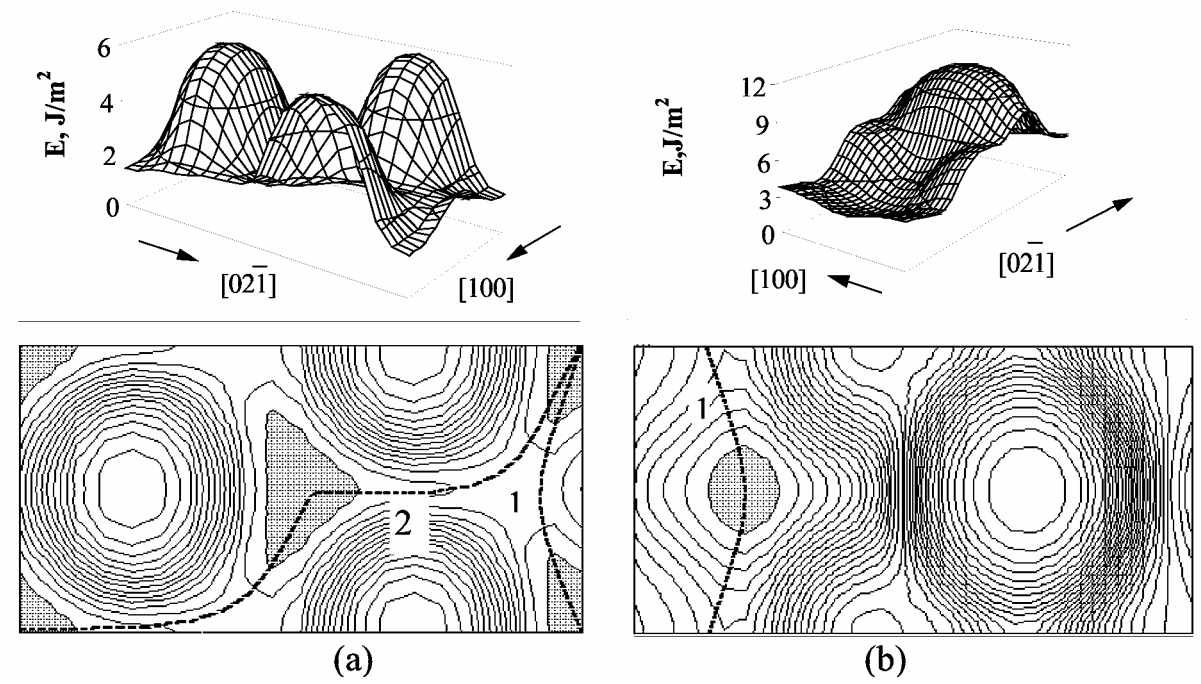

Fig.4. The γ-surfaces and contour plots their relief for the GB [100](012) in Al (a) and Fe (b) after atomic relaxation. Shaded areas - minima of energy. The dashed lines show trajectories of the GB sliding 1- along $[\bar{1}\,00]$, 2- along $[\bar{1}\,2\,\bar{1}]$

The shift along the Z-axis can be used for evaluation of GB exess volume. Exess volume (Δv was determined as $\Delta v/v_0=d/d_0-1$, where v_0 is volume of ideal crystal, d_0 is an interplane distance in an ideal lattice, d is a changed interplanar distance in the GB core. The calculated values of exess volume are listed in table 1. In Al the rigid relaxation takes place only as a result of exess volume, in Fe the exess volume is smaller, but there is a shift in the plane of boundary.

In Fig.4 the γ- surfaces of GB for Al and Fe after a full relaxation are shown. The mutual position of maxima on a γ-surface corresponds to the positions of atoms in a plane unit cell (Fig.2). The minimum determines a stable state of GB. The values of energy EA and the value of displacement after the full relaxation are listed in table 1. Full relaxation reduces GB energy additionally, however value of displacement vector f does not vary. Values of the GB energy, defined after full atomic relaxation, are equal to Al and Fe 880 and 1088 mJ/m^2 respectively. These values are satisfactory for Al and overstated for Fe, in comparison with experimental measurements [10], which proves the rigidity of the used potential for Fe.

The analysis of the γ-surface allows to determine GB sliding variants. GB sliding represents the transition of GB from one stable state to the other. The shift is carried out by the optimal trajectory and passes through the saddle point. Energy of a saddle point gives value of the potential GB sliding barrier. In Fig.4 the GB sliding trajectory is shown by a dashed line. In Al it is possible to select two directions of the GB sliding: $[\bar{1}00]$ and $[\bar{1}2\bar{1}]$, in Fe - there is only one $[\bar{1}00]$. The energy profiles of the γ- surface for GB sliding are shown in Fig.5. It is visible, that for the tilt GB [100] (012) GB sliding is connected with significant of energy consumption. For Al the value of potential barrier in the direction $[\bar{1}00]$ is little bit higher, than in the direction $[\bar{1}2\bar{1}]$, i.e. the preferable direction of GB sliding in Al is direction $[\bar{1}2\bar{1}]$. However, it is necessary to point out, that the data given in the Fig.5 show the energy value at displacement of grain as a whole. The GB sliding by means of GB dislocations can reduce the value of a potential barrier considerably. The Burgers vectors of GB dislocations are determined by the vector of shift from one minimum to the other. For Al the GB dislocations are possible with the

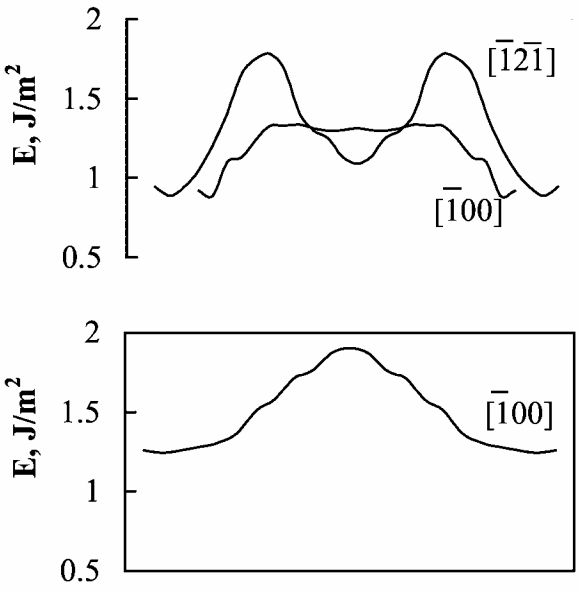

Fig.5. Profiles of the γ-surface along a trajectory of a shift at the GB sliding in Al and Fe. The directions of a shift are marked in square brackets

Burgers vectors $a[\bar{1}00]$ and $a[\bar{1}2\bar{1}]/2$. For Fe the Burgers vector is $a[\bar{1}00]$.

4. Conclusion

The computer simulation of the GB Σ=5[100](012) in Al and Fe has shown, that the GBs in the CSL model are unstable. The stabilization is achieved by the additional displacement of one grain relatively to the other by some vector f. In Al the displacement takes place in the direction of a normal plane of defect, in Fe both in normal and in parallel directions. The shifts normal to the boundary planes form exess volume at the GB equal to $0{,}28v_0$ and $0{,}04v_0$ for Al and Fe respectively. The calculations of the GB γ-surfaces in Al and Fe have shown, that there is no satisfactory accord between a potential relief in the GB plane and the DSC lattice. The basic vectors of DSC lattice do not allow to find steady GB states and to define the GB sliding directions. The analysis of γ-surface of the relaxation GB has shown, that there are directions of the facilitated GB sliding. In Al the directions are $[\bar{1}00]$ and $[\bar{1}2\bar{1}]$, in Fe - $[\bar{1}00]$.

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