THE RESEARCH OF GRAIN BOUNDARY SLIPPING AT THE TILT BOUNDARIES IN AL

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The computation simulation of atomic structure of tilt GBs in Al is carried out in this work. Special tilt boundaries with the axis of disorientation [100] and [110] were investigated. It was held the investigation of energetical relief of Peierls, appearing at the shear of one grain relatively to the other along the grain boundary plain. The investigation was held by the method of construction of γ-surface. Atomic relaxation of the crystal was made by the method of molecular statics. Interatomic interaction was approximated by Morse pair potential. The relaxed model, in which the atoms were allowed to displace outside the site under the action of interatomic forces, was used. The initial structure for γ-surface construction was chosen in the model of coincide site lattice. The investigations of γ-surfaces are shown that GB has several stable states. Reorganization of structure of GBs can be pass through intermediate metastable states. The relief of γ-surface is used for determination of Burgers vectors and directions of movement of grain boundary dislocations. The directions of slipping and Burgers vectors of grain boundary dislocations were found for investigating boundaries.

1. Introduction

Numerous researches of the latest years have shown that grain boundaries (GB) are important elements of defect structure, influencing on many properties of polycrystals. The number of fundamental processes is in the basis of this influence, including, for example, grain boundary slipping [1]. It is supposed, that grain boundary slipping takes place in the result of moving of specific grain boundary dislocations (GBD), but the nature of these dislocations, their characteristics have been studied a little. Experimentally discovered shears at GB and ordered structure of boundaries testify to the necessity of the presence of specific grain boundary dislocations [2, 3].

As it is known, GBD can be proper and carried into ones [1]. Proper grain boundary dislocations are necessary, for example, for ensuring of the declination of GB misorientation from special one, that is why they are not the defects of proper GB structure. Burgers vectors of GBD are usually determined in the model of coincidence site lattice (CSL). In this model, proper GBD have Burgers vectors, defined by the displacement shift complete lattice and grain boundary shift lattice [4, 5].

Carried into GBD can appear in GB by the effect of some grain boundary source or at the interaction of lattice dislocations with GB [6]. Burgers vector of carried into GBD is the subject of the discussion. It is often supposed that it also can be determined by basis vectors of displacement shift complete lattice and grain boundary shift lattice. This supposition is based on the fact, that Burgers vectors of lattice dislocation can be represented by the sum of basis vectors of displacement shift complete lattice, that is why lattice dislocation can break down in the boundary at GBD with Burgers vectors, also the vectors multiple to the basis vectors of displacement shift complete lattice. For determination of Burgers vectors of carried into GBD, it can be used γ-surface, which looks like energetic relief, appearing at the shear of one grain relatively to the other along the plain of GB [7]. The relief of γ-surface corresponds to Peierls relief and it is often used for the analysis of dislocations moving in the ideal lattice [8]. The construction of γ-surface can be used for determination of Burgers vectors of GBD and shear directions of one grain relatively to the other.

2. Method of calculation

Computer simulation of the atomic structure of GB in Al was made in the given paper. Special tilt boundaries Σ=17[100](014) and Σ=9[110](114) were studied. Interatomic interaction was described by pair empiric Morse potential and it was taken into account the interaction in three coordination spheres. The parameters of the potential were determined by equilibrium properties of Al (lattice constant, cohesive energy, elastic constant). Energy of GB was defined as the difference between the energy of defect crystal and the energy of an ideal one. The calculation of GB energy was made by the method of hard three-dimensional relaxation, which allows to make the displacement of grain one relatively to the other as parallel, so

perpendicular to the plain of boundary. The initial structure of GB for the construction of γ-surface was constructed in the framework of the model of CSL.

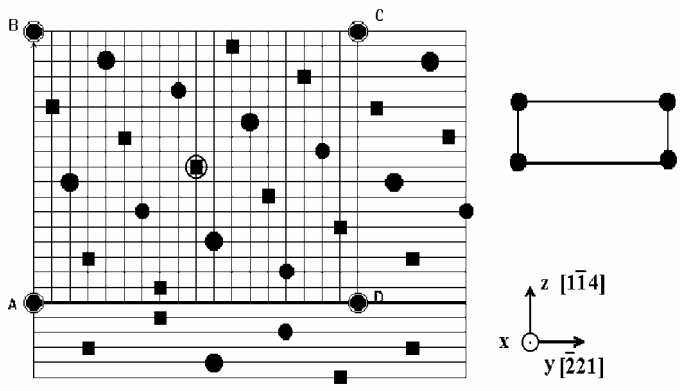

Fig.1. The structure and the form of unit cell of the grain boundary Σ=9[110](114), ABCD - unit cell of CSL

The research of Peierls energetic relief, appearing at the shear of one grain relatively to the other, was held in this paper. Peierls relief at the movement of GBD was calculated by the method of the construction of γ-surface.

Fig.1. shows the structure and the form of unit cell of GB Σ=9[110](114). Coordinate axes were chosen to make the axis x be parallel to the axis of GB misorientation, the axis y was parallel to the plain of GB (114), axis z was perpendicular to the plain of GB (AD – the plain of GB). Fig.1. demonstrates two atomic plains [110]. The atoms of upper plain are marked by dark circles, the atoms of lower plain – by the squares. The atoms, marked by the circles, are situated at the sites of CSL. The research of GB was held with the help of the construction of γ-surface for one structural unit because the investigating boundaries of grains consist of recurring elements.

3. Results and discussion

Fig.2. and 3 show γ-surfaces, their projections on the plain of defect and energetic profiles of γ-surfaces at grain boundary slipping, received for investigating boundaries. The calculated γ-surfaces has complicated relief. Main elements of the relief are maximums, minimums and saddle points. Maximums at γ-surfaces correspond to the positions of atoms in the plain of boundary, minimums define stable and metastable states of GB (stable state is marked by the letter S, metastable states are marked by the letters of Greek alphabet - α, β and others). Saddle points define the value of energetical barrier and the direction of possible transitions of GB from one state into another at grain boundary slipping. The arrows in fig.2 show the directions of possible grain boundary slipping. The analysis of γ-surface shows, that grain boundary slipping can be realized as by the

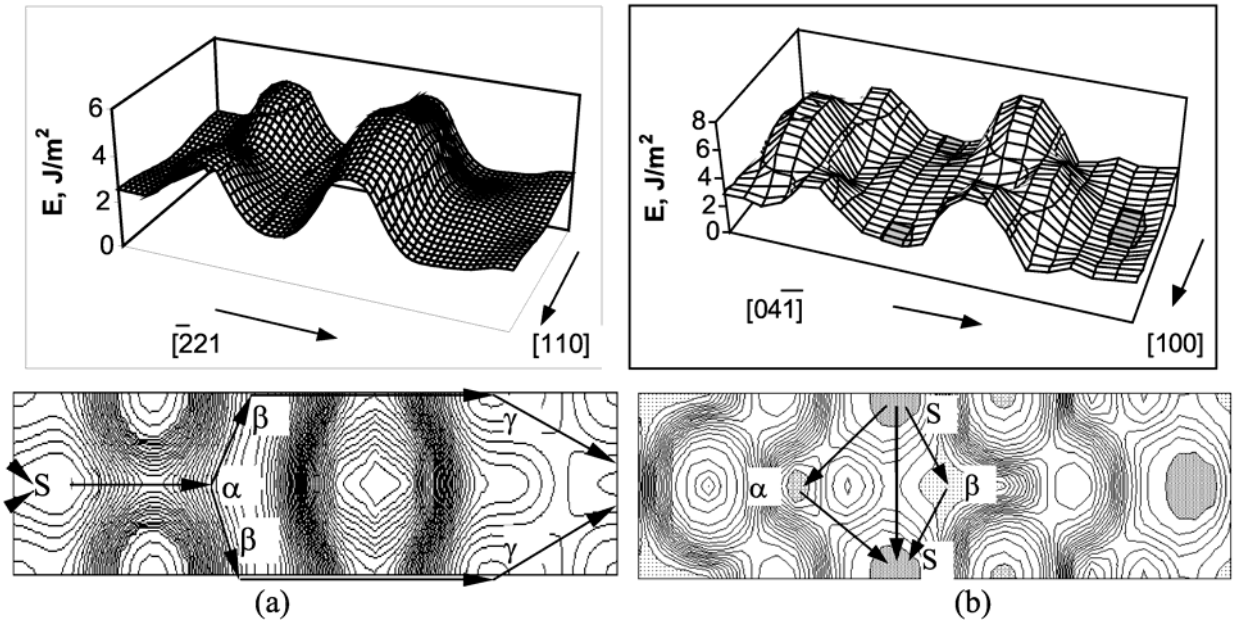

Fig.2. γ-surfaces and their projections on the plain of defect: a) GB Σ=9[110](114), b) GB Σ=17[100](014)

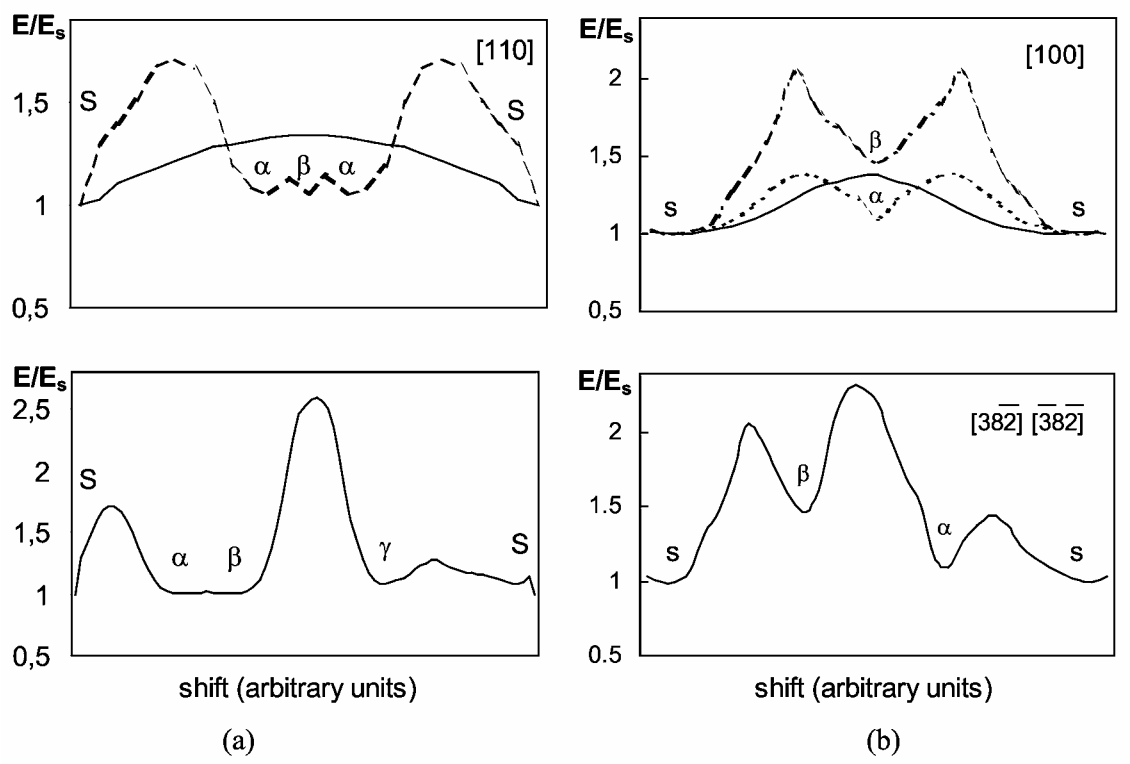

Fig.3. Energetical profiles of γ-surfaces at grain boundary slipping: a) GB Σ=9[110](114), b) GB Σ=17[100](014)

transition from one stable state into another, so by metastable state. The reactions of reconstruction at grain boundary slipping can be written by the following:

$$S \rightarrow S; \quad (1)$$

$$S \rightarrow \alpha \rightarrow S. \quad (2)$$

Grain boundary slipping from one stable state into another takes place at the movement of full GBD. If the shear of grains realizes through interstitial states (α, β and others), full dislocation dissociates into partial ones. Potential barrier of GB transition from one state into another is of great importance for the proceeding of grain boundary slipping. The analysis of energetical profiles shows, that anisotropy of slipping takes place. The least potential barrier for GB Σ=17[100](014) realizes in the direction [100], for the grain boundary Σ=9[110](114) – in the direction [110].

The structure of GB Σ=9[110](114) in the CSL model is unstable, because it corresponds to the maximum at γ-surface. There are also two minimums else, besides state, they correspond to metastable states α and β, the transition in these states requires relative displacement of grains. The analysis of energetical profiles of γ-surface shows, that the least potential barrier is in the direction [100]. The most probable grain boundary slipping for GB (014) is grain boundary slipping through interstitial state α in correspondence with the reaction (2). The shear through interstitial state α means, that full GBD, having Burgers vector **b**=a[100], dissociates into partial ones. From the analysis of γ-surface relief, it can be written the following dislocation reactions for GBD:

$$a\,[100] \rightarrow \frac{a}{8}[4\,\bar{4}\,1] + \frac{a}{8}[4\,4\,\bar{1}]. \quad (3)$$

The structure of the grain boundary Σ=9[110](114) in CSL model is not stable, because the maximum corresponds to it at γ-surface. There is one stable state of the boundary (S) and four metastable states (α, β, γ, δ). The analysis of γ-surface of the grain boundary Σ=9[110](114) shows, that grain boundary slipping takes place only by partial dislocations in correspondence with the reaction (2). Dislocation reaction can be written as follows:

$$\frac{a\sqrt{2}}{2}[110] \rightarrow \frac{a}{16}[\bar{1}\bar{0}\,\bar{6}\,1] + \frac{a}{16}[10\,6\,\bar{1}]. \quad (4)$$

In the result of the GB research, Burgers vectors of GBD were determined by the method

of the construction of the energetical γ-surfaces. Burgers vector of the GBD for the GB Σ=17[100](014) was equal to **b**=$\frac{a}{8}\langle 441\rangle$, for GB Σ=9[110](114) it was equal to **b**=$\frac{a}{16}\langle \bar{1}0\ \bar{6}\ 1\rangle$.

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