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The Structure of (001) CSL Twist Boundaries in fcc Metals

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Abstract

Computer simulation techniques based on discrete lattice approach and empirical many-body potentials have been used to study the structure and energy of $\Sigma = 5$, and $\Sigma = 13$ coincident site lattice (001) twist boundaries in three fcc metals. Energy computed for $\Sigma = 5$ boundary in copper is 17.5 % less than the earlier result obtained by using pair potential. However the present calculations of twist boundary energies are somewhat higher than the results obtained using embedded atom method.

1. Introduction

The understanding of the atomic structure of grain boundaries is a necessary precursor for the development of microscopic theories of boundary characteristics. For this reason the grain boundary structures have been investigated by many research workers. Number of experimental techniques have been applied to determine the structure of grain boundaries [1-6]. The relationship between physical properties and structure of the grain boundaries have also been theoretically investigated [7-9]. The Coincident Site Lattice (CSL) model [10], widely used, focuses on the misorientation relationship between the two halves of a bicrystal in terms of rotation of two interpenetrating crystal lattices. The inverse density of CSL sites Σ is mostly used to correlate the structural properties of the boundaries.

The crucial decision to simulate a specific type of defects, in crystal, is the choice of an appropriate interatomic potential. All the potentials increase sharply for decreasing distance. The grain boundary energy is almost completely controlled by the strong repulsion between the boundary atoms which are at distances closer than those in the perfect

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crystal. Many-body potentials for fcc metals have been developed by Ackland et.al. [11], according to which the energy of the ith atom is:

$$U_i = \frac{1}{2}\sum_j V(r_{ij}) - \left[\sum_j \phi(r_{ij})\right]^{1/2},$$

where r_{ij} is distance between atoms $i\&j$. The summation extends to all atoms of the system. The six cubic spline pair potential function $V(r)$ is given as:

$$V(r) = \sum_{k=1}^{6} a_k(r_k - r)^3\ H(r_k - r)$$

and two cubic spline embedding cohesive potential ϕ is:

$$\phi(r) = \sum_{k=1}^{2} A_k(R_k - r)^3\ H(R_k - r),$$

where r_k, R_k are knot points and $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x \geq 0$. The coefficients $a_1, a_2, \ldots, a_6$, A_1 and A_2 were determined by fitting to the lattice parameter a, the cohesive energy E_c, the elastic constants C_{11}, C_{12} and C_{44}, the relaxed vacancy formation energy E^f and the stacking fault energy. The values of these coefficients for various fcc metals are given in reference [11].

The possible structure of twist boundaries in copper have been simulated by Wolf [7, 9] employing the Embedded Atom Method (EAM) and Lennard-Jones (LJ) potential. Unfortunately, both of the potentials give zero energy for the $\Sigma = 3$ (111) twist boundary. Many-body potentials, described above, have successfully been applied to simulate the structure and energy of twin boundaries [12], twin-vacancy interaction [13] and various (111) twist boundaries [14]. The $\Sigma 3(111)$ twist boundary energy in gold, computed by this potential, is 31.71 mJ/m^2 [14] which lies within the experimental values $30 - 40 mJ/m^2$ compiled by Gallagher [15]. Therefore it was decided to simulate (001) twist boundaries using the many-body potential proposed by Ackland et.al. [11]. The present paper includes low energy structures of $\Sigma = 5, \Sigma = 17$ and $\Sigma = 13$ CSL (001) twist boundaries corresponding to misorientation angles of $36.87°, 28.07°$ and $22.62°$ in copper, silver and gold. The computational procedures adopted and results obtained are described in the next section while significance of these results is discussed in the last section.

2. Computational Method and Results

The model fcc crystal used for simulation was generated in the form of a square prism with three mutually perpendicular axes. The atoms in the computational region were free to move under the applied many-body potential. This computational region was surrounded by a thick mantle region such that the outer atoms of the computational cell have full quota of their neighbors. Depending on the boundary conditions, the atoms

of the mantle region may or may not be allowed to move. The appropriate boundary conditions for simulation of planner defects, are to keep the faces parallel to the interface fixed while periodic boundary conditions be imposed on rest of the faces.

A twist boundary can readily be introduced into the model without altering its shape. In practice, the twisted model was generated from a single crystal by displacing the non-CSL sites on one side of the interface through minimum magnitudes. The periodic boundary conditions normal to the interface effectively simulate the infinite twist boundary, thus giving the more realistic results.

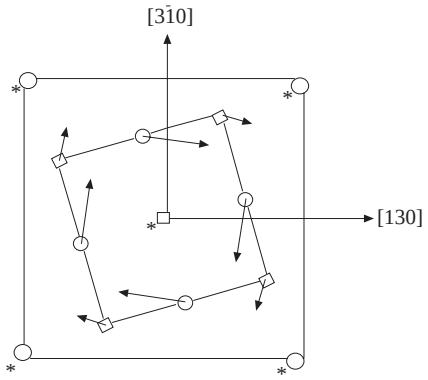

Figure 1. Arrangements of atoms in the 1st and 2nd neighboring planes above the boundary, represented by squares & circles, of the twisted crystal model. The arrows represent the components of displacements (magnified ten times) parallel to (001) during relaxations. The CSL sites are indicated by *.

2.1. $\Sigma = 5$ (001) Twist Boundary

In order to simulate $\Sigma = 5(001)$ twist boundary, the model crystallite constructed was a rectangular block of 300 moveable atoms surrounded by 4086 atoms in the mantle. The computational cell was comprised of 10(130), 10(3$\bar{1}$0) and 60(001) planes. The faces (130) and (3$\bar{1}$0) were subjected to periodic boundary conditions while (001) faces were simulated under fixed boundary requirements. The twist boundary was generated by shuffling of non-CSL atoms within (001) planes by proper magnitudes, in one half of the model.

In order to obtain minimum energy configuration the model was allowed to relax. Studying the resulting configuration of the atoms, two types of distinct displacements for CSL and non-CSL are noted to occur. The displacements for CSL sites are all perpendicular to the (001) plane. However, displacements for the non-CSL sites have components both parallel and normal to this plane. Equal and opposite displacements arose for equivalent sites on both sides of the interface. The magnitude of displacements for the atoms in the plane adjacent to the boundary are almost four times as compared to the displacements of the atoms in the next neighboring planes. The displacements occurred during

relaxation in the adjacent two planes of one side of the interface are shown in Figure 1. Of course the next neighboring planes were found to have insignificant displacements. The non-CSL atoms of both the planes are rotated clockwise about CSL sites of the 2nd plane. The relaxed structure of the Σ5 twist boundary in copper is shown in Figure 2.

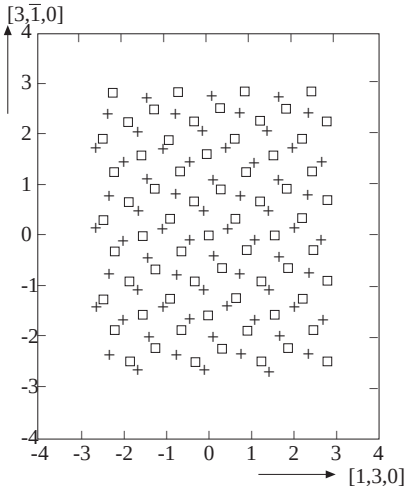

Figure 2. A relaxed structure of Σ5 twist projected on the (001) boundary plane. Two atomic planes just below the boundary are indicated by + and .

In order to eliminate compressive strain around the boundary, a plot of displacements of individual (001) planes normal to the interface was sketched. The appropriate amount of magnitude by which the grains must be moved apart was determined [12] to be 0.128a, 0.118a and 0.116a for copper, silver and gold, respectively. After applying the above expansions, the twist boundary energies for three metals are found to be 998.75, 710.58 and 726.67 mJ/m^2.

2.2. $\Sigma = 17$ (001) Twist Boundary

To study $\Sigma = 17(001)$ twist boundary, a rectangular crystallite of atoms with $34(4\bar{1}0)$, 34(140) and 32(001) planes was generated. Sufficient number of mantle atomic planes were added on all sides of the computational model. The faces $(4\bar{1}0)$ and (140) were kept under cyclic boundary conditions. The (001) faces being parallel to the boundary were simulated with fixed atoms in the mantle region. The twist boundary was again created by minimum atomic shuffle, of non-CSL atoms, at the middle of the model in [001] direction.

Minimum energy configuration of the twisted crystallite obtained by relaxing it through the many-body potential is shown in Figure 3. For the CSL and non-CSL sites, here again, two distinct types of displacements were noted to occur. Equal and opposite displacements occurred for equivalent sites on both sides of the interface are nearly twice those in

the next neighboring planes. The non-CSL atoms moved clockwise around the CSL sites. The expansions of the model, to eliminate the strain at the boundary, in [001] direction were calculated to be 0.106a, 0.100a and 0.100a for copper, silver and gold respectively. The boundary energies so obtained are 910.34, 667.17 and 655.49 mJ/m^2, respectively, for the three metals.

2.3. $\Sigma = 13(001)$ Twist Boundary

To simulate the $\Sigma = 13(001)$ twist boundary a rectangular crystallite of atoms bounded by $(5\bar{1}0)$, (150) and (001) faces, was generated. The computational cell of moveable atoms consisted of $26(5\bar{1}0)$, 26(150) and 60(001) planes. The mantle atoms on the (001) faces were kept fixed while those on the remaining faces were simulated under periodic boundary conditions. The twist boundary was created at the middle of the model in [001] direction by applying minimum atomic shuffle of non-CSL sites on one half of the model.

The model was allowed to relax to attain the minimum energy configuration (Figure 4). The results reveal that two distinct types of displacements for CSL and non-CSL sites occur as in the cases of $\Sigma = 5$ and $\Sigma = 17$ twist boundaries. The large displacements are associated with atoms in the first plane, whereas the next planes observe minor displacements. It has further been noted that the non-CSL atoms of the 1st and 2nd planes are rotated clockwise about CSL sites of the 2nd plane.

The compressive strain near the boundary was removed through expansions of the model by 0.116a, 0.103a and 0.102a for copper, silver and gold respectively in [001] direction. The twist boundary energies for these metals, after applying above expansions, are 834.37, 602.14 and 585.31 mJ/m^2, respectively.

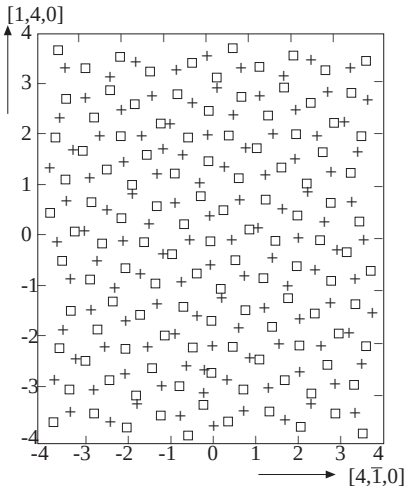

Figure 3. Relaxed structure of the two neighboring planes of the Σ17 twist boundary projected on the (001) plane.

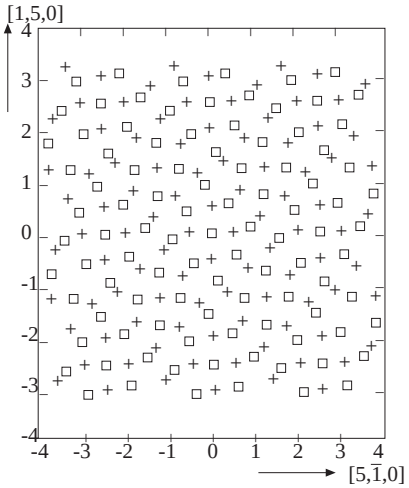

Figure 4. A relaxed structure of Σ13 twist projected on the (001) plane.

3. Discussions

The atomic structure of (001) twist boundaries have been explored with misorientation angles of $36.87°, 28.07°$ and $22.62°$ corresponding to $\Sigma = 5, \Sigma = 17$ and $\Sigma = 13$. The relaxed boundary structures are shown in Figures 2 to 4 and the energies obtained are summarized in Table 1. The results provide sufficient structural information. The displacements occurred during relaxation are all plausible in terms of the structure of the interface. Non-CSL atoms of the planes adjacent to the boundary move apart during relaxation as they are much closer than the nearest neighbor separation. The results are acceptable because of the fact that atoms located at crystallographically equivalent sites are displaced identically. They are also consistent in nature with the results published earlier for other twist boundaries [7-9, 14].

Table 1. (001) twist boundary energies in units of mJ/m^2

Type	θ (deg)	Copper	Silver	Gold
$\Sigma = 5$	36.87	998.75	710.58	726.67
$\Sigma = 17$	28.07	910.34	667.17	655.49
$\Sigma = 13$	22.62	834.37	602.14	585.31

Bristowe and Crocker [8] have used non-equilibrium semi-empirical two-body interatomic potential to calculate the structure and energy of $\Sigma = 5$ (001) twist boundary in copper. They found a volume increase of about 0.08[001]a and a boundary energy of 1210 mJ/m^2. The present results for the same boundary are, 0.13[001]a and 998.75 mJ/m^2, respectively. In the present calculations a four times larger model has been used and more sophisticated many-body potentials are employed, which have already been successful in the simulation of several twin and twist boundaries [12-14]. The energy computed is 17.5

% lower than that of Bristowe and Crocker [8]. For the same boundary Wolf [7] has obtained a volume increase of 0.12[001]a, and the boundary energy of $700mJ/m^2$ using EAM and LJ potentials. Also for $\Sigma = 17$ (001) and $\Sigma = 13$ (001) twist boundaries in copper, he has obtained about 28 % lower energies than our present results. This is due to inherent problem with both EAM and LJ potentials that both give zero (111) stacking fault energy. Therefore the present results could be considered more reliable.

In general twist boundary energies for copper are lower than silver and that of silver are lower than the gold. There is only one exception to be noted from the result summarized in Table 1, i.e. $\Sigma = 5$ silver energy is lower than for the same boundary in gold. Also, silver and gold boundary energies differ by less than 3 %.

Acknowledgement

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