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ENERGETICS AND STRUCTURAL PROPERTIES OF TWIST GRAIN BOUNDARIES
 IN Cu

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Introduction

Structural and energetics properties of atoms near a grain boundary are of great importance from theoretical and experimental standpoints. From various experimental work it is concluded that diffusion at low temperatures at polycrystalline materials take place near grain boundary. Experimental and theoretical results also indicate changes of up to 70% in physical properties near a grain boundary. The Embedded Atom Method (EAM) (1) calculations on structural properties of Au twist grain boundaries (2) are in quite good agreement with their experimental counterparts. The EAM is believed to predict reliable values for the single vacancy formation energy as well as migration energy. However, it is not clear whether the EAM functions which are fitted to the bulk properties of a perfect crystalline solid can produce reliable results on grain boundaries.

One of the objectives of this work is to construct the EAM functions for Cu and use them in conjunction with the molecular static simulation to study structures and energetics of atoms near twist grain boundaries $\Sigma 5$ and $\Sigma 13$ in Cu. This provide test of the EAM functions near a grain boundary. In particular, we determine structure, single vacancy formation energy, migration energy, single vacancy activation energy, and interlayer spacing as a function of distance from grain boundary. Our results are compared with the available experimental and theoretical results from grain boundaries and bulk.

Methodology

Interatomic pair potentials suffer from two major problems, zero Cauchy pressure, i.e., $C_{11}-C_{12}=0$, and equality of single vacancy formation energy E_{1v} and cohesive energy E_c . In practice, for most crystals $C_{11} \neq C_{12}$ and $E_{1v} \neq E_c$. To overcome these and other shortcomings of pair potentials the EAM potentials are developed. In the EAM, the major contribution to energy of each atom is due to the embedding energy which is supplemented by a two body potential. The embedding energy of an atom can be interpreted as the energy that is required to embed that atom in the electronic charge produced by the other atoms in the crystal. The two body potential ϕ can also be interpreted as the electrostatic interaction between cores of embedding atom and atoms of crystal. Energy of atom i in the EAM formalism can then be written as,

$$E_i = F_i(\rho_i) + 0.5 \sum_{j \neq i} \phi_{ij}(r_{ij})$$

where E_i is the energy of atom i , F_i is the embedding energy of atom i , ϕ_{ij} is the two body potential between atoms i and j , r_{ij} is the

interatomic distance between atoms i and j , and ρ_i is the charge density at site i due to atoms in other sites. One of the assumptions in the EAM approach is that ρ_i is superposition of atomic charge densities from all the other sites,

$$\rho_i = \sum_{j \neq i} \rho_j^a$$

where ρ^a is the atomic charge density.

F and ϕ are determined by considering their functional forms and finding their parameters by fitting to the bulk properties of crystalline solid (3).

In our calculations, we have employed the EAM functions of Cu along with the molecular static routine to study structures and energetics of twist grain boundaries. In a molecular static simulation, total energy of the system is minimized with respect to positions of atoms. In any energy minimization approach extreme caution should be taken that final state of the system has the lowest energy (i.e., global minimum).

Results

a) single vacancy formation energy

Our $\Sigma 5(\theta=36.87)$ and $\Sigma 13(\theta=22.62)$ twist grain boundaries are comprised of 14 fcc(001) atomic layers, 80 atoms per layer, and with half of the layers rotated with respect to the (001) axis by an angle θ . A vacancy is created in a desired site and the single vacancy formation energy E_{1v}^f is calculated using,

$$E_{1v}^f = E(N-1, 1) - E(N, 0)$$

where $E(N-1, 1)$ is the total energy of a system of N atomic sites with $N-1$ sites filled and 1 site vacant and $E(N, 0)$ is the energy with all N sites filled. Our results for E_{1v}^f are plotted in Fig.(2).

b) Migration and activation energies

Various migration paths for vacancy is considered (look at Fig. 1) by moving the atom through the desired path and allowing it to relax in the plane perpendicular to the path. All the other atoms are allowed to relax without any constraint. Total potential energy of the system is then calculated as a function of migrating

distance. Our results for migration energies are reported below and plotted in Fig.(2):

$\Sigma 5$	$\Sigma 13$
$E_{1m} = 0.018$ ev, path 1	$E_{1m} = 0.037$ ev, path 1
$E_{1m} = 0.050$ ev, path 2	$E_{1m} = 0.018$ ev, path 2
$E_{1m} = 0.087$ ev, path 3	$E_{1m} = 0.016$ ev, path 3
$E_{1m} = 0.7$ ev, path 4 (bulk)	$E_{1m} = 0.7$ ev, path 4 (bulk)

Single vacancy activation energy $Q = E_{1v}^f + E_{1m}$ is calculated and plotted in Fig.(2).

c) Interlayer spacing across a $\Sigma 5$ grain boundary

Total energy of the grain boundary lattice described in part (a) is minimized using our molecular static code and interlayer spacing is calculated and plotted in Fig.(3).

Summary and conclusion

Our work can be summarized as follows:

- a) Vacancy formation energy is shown to be directly correlated to the degree of coincidence.
- b) Single vacancy activation energy near the grain boundary is about 60% lower than its corresponding value in the bulk.
- c) Vacancy migration energy near a $\Sigma 5$ or $\Sigma 13$ grain boundaries is about 0.1 ev which is much smaller than its corresponding bulk value of ~ 0.7 ev.
- d) Interlayer spacing at a $\Sigma 5$ grain boundary is enhanced by a factor of about 17% as compared to its bulk value.

References

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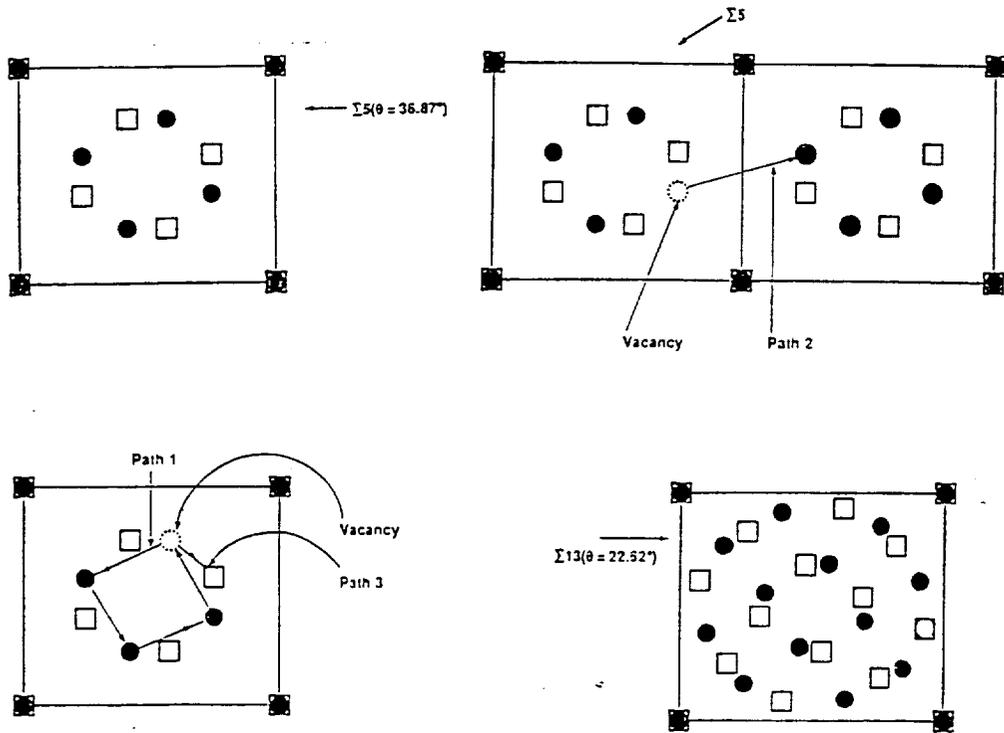
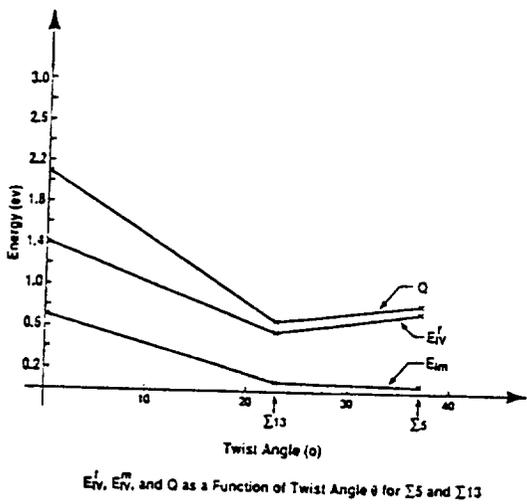


Fig. (1)



E_V^I , E_V^M , and Q as a Function of Twist Angle θ for $\Sigma 5$ and $\Sigma 13$

Fig. (2)

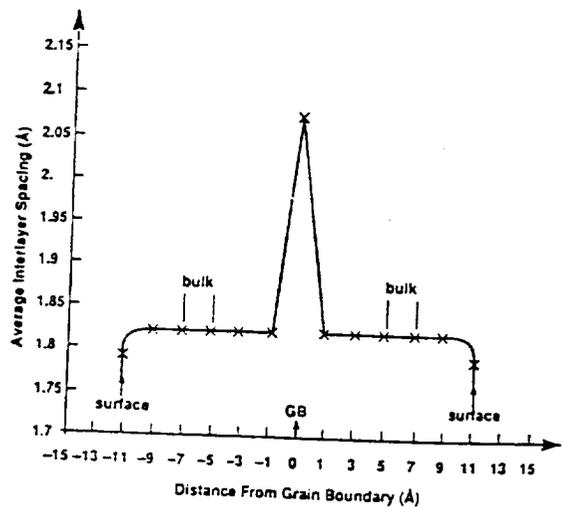


Fig. (3)