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CUBIC [001] TWIST CSL GRAIN BOUNDARIES STUDY BY MEANS OF RANDOM WALK(1)

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Abstract - The random walk procedure has been applied on some typical relaxed CSL twist grain boundaries. The relaxation has been achieved by means of the Molecular Dynamics method, applied on the CSL computational cells. Some of the random walk parameters are discussed and the information dimension is examined as a function of the rotation angle $\theta$. The remarkable anisotropy observed in the parameters between the grain boundary and the bulk is common to many dynamical properties of the grain boundaries.

1. INTRODUCTION

With the exception of the twin Grain Boundaries (GB) almost all the others GBs are, in some way, a disorder region of the bicrystal. A model of great current interest for the GBs studies is the Coincidence Site Lattice (CSL) model. The knowledge of the CSL, which might exist in a given bicrystal orientation, extends the relationship between the structure and the properties of the GB to a quantitative measure. In fact a measure of the order existed in a GB can be defined by means of the CSL and also it provides adequate computational cells for many computational procedures concerning the GBs behavior /1/.

Thus the equilibrium configurations of many different materials have already been studied by this model and the corresponding relaxed energies have been estimated /2/. Transport phenomena have also been studied by means of the CSL computational cells by using the Molecular Dynamics (MD) method /3/.

In this paper results are reported from the study of CSL GBs on the basis of the random walk procedure. The relaxed CSL unit cells are obtained by the MD procedure for low to moderate misorientations and four different CSL multiplicities $\Sigma$ are examined.

2. A CSL BICRYSTAL

Imagine two identical crystals and bring them in contact by a common plane. Rotate the one with respect to the other by a special rotation $R$ and let them to relax. Depending on the choice of the rotation matrix $R$ there is always a fraction $1/\Sigma$ of lattice points whose coordinates are identical in both crystals. Their density $1/\Sigma$ is a function of the rotation axis $r$ and the rotation angle $\theta$ /4/. These points define the so-called CSL which can be thought as a superlattice containing the two lattices. The unit cell of the CSL can be easily defined by the properties of the rotation matrix $R$ /5/.

The boundary region between the two crystals could be any but in this report we deal with a special type of GBs known as twist GBs, i.e boundaries between two crystals whose mutual orientation is described by a rotation about the [001] axis perpendicular to the boundary. The relaxed properties of these GBs have been systematically studied from experimental and theoretical point of view /6/.

The models used in the present work have the following characteristics: Their computational cell consists of eight successive (001) planes with cross-sections defined by the unit cell of the CSLs. The GB is located in the middle of the computational cell. The corresponding CSL multiplicities are $\Sigma=5$, 13a, 25a and 61a. They are allowed to relax by using the MD procedure /7/. The potential used is the L-J potential for Ne. Displacements of the atoms appear in the first planes from both sides of the boundary and they are progressively reduced in the bulk region and finally they are diminished to the outer planes. As the density of the CSL points is reduced the number of the displaced atoms increases both in the bulk and in the GB region. The symmetry of the relaxed CSL unit is that of the initial structure.

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3 - INFORMATION DIMENSION

The information dimension $D_i$ has been introduced recently for the study of transport properties in homogeneous and random systems /8/. Consider a random walk on the discrete lattice space and let $P_k$ be the probability of the walker to visit the $k$-th site; then by definition:

$$D_i = \frac{I_n}{\ln(n)}$$

where

$$I_n = -\Sigma P_k \ln P_k$$

and $n$ is the number of discreet steps. The sum of the equation (2) is extended over the number $S_n$ of distinct sites visited at least once by the random walker. For every finite scheme, i.e. a set of values $P_j = 1, \cdots, S_n$ ($P_j > 0, S_n < n, \Sigma P_j = 1$) the function $-\Sigma P_k \ln P_k$ describes a state of uncertainty. Furthermore, for fixed $n$ values, it is obvious that the scheme with the greatest uncertainty is the one with equally probable events, i.e. $P_k = 1/S_n$. By substituting these occupation probabilities in relation (2) we deduce:

$$I_n = -\Sigma (1/S_n) \ln (1/S_n) = \ln S_n$$

or

$$D_i = \frac{\ln S_n}{\ln(n)} (3)$$

by using relation (1). Relation (3) means that the information dimension for a finite scheme of $S_n$ equally probable events is equal to the half of the spectral dimension $D_s$, i.e. $D_i = D_s/2$. Thus for a given finite scheme, but not the one of the equally probable events of relation (3), someone should expect that the value of $D_i$ is a function only of the scheme.

However, de Arcangelis et al /9/ have also recently proved on the basis of all related exponents theory that $D_i$ tends to the spectral dimension $D_s/2$ as $n$ tends to infinity. This analytical treatment shows clearly that $D_i$ belongs in the same class as the exponent $D_s$. However, for all practical finite purposes, $D_i$ must have a well defined value /10/. Thus someone may readily see that $D_i$ is, in some respect, an analytical expressed form of the spectral dimension with well defined properties. It is a function of the occupation probability $P_k$ and of course its numerical value for every finite scheme characterizes the nature of the particular space in which the random process is performed /11/.

4 - COMPUTATIONAL PROCEDURE AND RESULTS

On a model bicrystal with about $10^5$ atoms the relaxed CSL unit cells have been repeatedly embeded. The random walk starts from a CSL point in the middle of the model. By considering the variation of the distance between the first nearest neighbors as a parameter the bonding percolation cluster has been examined, i.e. the continuous interconnection between atoms of the same distance /12/. There is a critical distance $d_c$ for which the grain boundary and the bulk material can be distinguished. We define this as the greatest distance which is less than the lowest distance existed in the unrelaxed material. The selection rule for the next time step is just this distance and multiple choices are decided by Monte Carlo method. All the experiments have been made on a 1000-steps walk and the random walk parameters have been taken after 1000 realizations. These parameters are the mean average bonding cluster size $<z_b>$, the GB mean average visits $<GB_v>$, the bulk mean average visits $<Bulk_v>$ and the $D_i$ parameter. In Table 1 results are given for four different $\Sigma$s examined.

<table>
<thead>
<tr>
<th>$\Sigma$</th>
<th>$\theta$</th>
<th>$&lt;z_b&gt;$</th>
<th>$&lt;GB_v&gt;$</th>
<th>$&lt;Bulk_v&gt;$</th>
<th>$D_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>36.87</td>
<td>29.4</td>
<td>970.4</td>
<td>29.6</td>
<td>.138137</td>
</tr>
<tr>
<td>13a</td>
<td>22.62</td>
<td>21.7</td>
<td>656.8</td>
<td>343.2</td>
<td>.215778</td>
</tr>
<tr>
<td>25a</td>
<td>16.26</td>
<td>35.7</td>
<td>651.8</td>
<td>348.2</td>
<td>.242040</td>
</tr>
<tr>
<td>61a</td>
<td>10.39</td>
<td>268.9</td>
<td>793.6</td>
<td>206.4</td>
<td>.339285</td>
</tr>
</tbody>
</table>
From these results the variation of all the parameters as a function of the value of $\theta$ is remarkable. Moreover the low dimensionality and the anisotropy between the GBs and the bulk properties is also obvious. This anisotropy is in accordance with the general GB behavior in the dynamical phenomena as it has been already pointed out /13/. The increase of the mean average bonding cluster size reflects the corresponding increase of the number of the displaced atoms. This increase becomes higher in the case of $\Sigma 61a$. Detailed examination of the occupation probabilities show a preference of the walker to visit the neighborhood of the CSL points. Experiments with a 10% variation of the distance show a tremendous variation in the mean average cluster size as well as in the $D_I$ value. The results of Table 1 correspond to the critical distance and the mean average cluster variation is followed by a reasonable variation of the uncertainty function $I_r$. This behavior becomes obvious from the values of the information dimension $D_I$. A plotting of $D_I$ as a function of $\theta$ given in Fig. 1, predicts a relation of the form $D_I = A\theta^a$, where $A$ and $a$ are constants of the order of unit. Finally, it should be noticed, from the values of the parameters $<\text{GB}_r>$ and $<\text{Bulk}_r>$, that the mean average number of visits is always in favor of the GB.

Fig. 1 - Grain boundary information dimension $D_I$ as a function of the rotation angle $\theta$ for the [001] twist GBs in Ne. Numerical values are given for the CSL multiplicities $\Sigma = 5, 13a, 25a, 61a$.

5 - DISCUSSION

In an attempt to corelate the GB microscopic geometrical properties with the macroscopic properties the random walk method has been used. Since the percolation problem applied to transport properties is not only a function of the distance but also of the properties of each place, our results concern only the effective geometrical form of the relaxed GBs examined. The most strict result of the present study is the variation of the information dimension $D_I$ as a function of the rotation angle $\theta$. Details concerning the site and bonding model applied in specify relaxed materials will appear elsewhere.

REFERENCES

/6/ Balluffi, R.W., Komem, Y. and Schober, T., Surf. Sci. 31 (1972) 68.
/7/ Doni, E.G. and Bleris, G.L., see paper in this Conf. Proc.