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Presented at the International Symposium (JIMIS-4) on Grain Boundary Structure and Related Phenomena, Minakaomi Spa, Japan, November 25-29, 1985

TRANSLATIONS AND STRUCTURE IN SYMMETRICAL TILT BODY-CENTERED-CUBIC GRAIN BOUNDARIES

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October 1985

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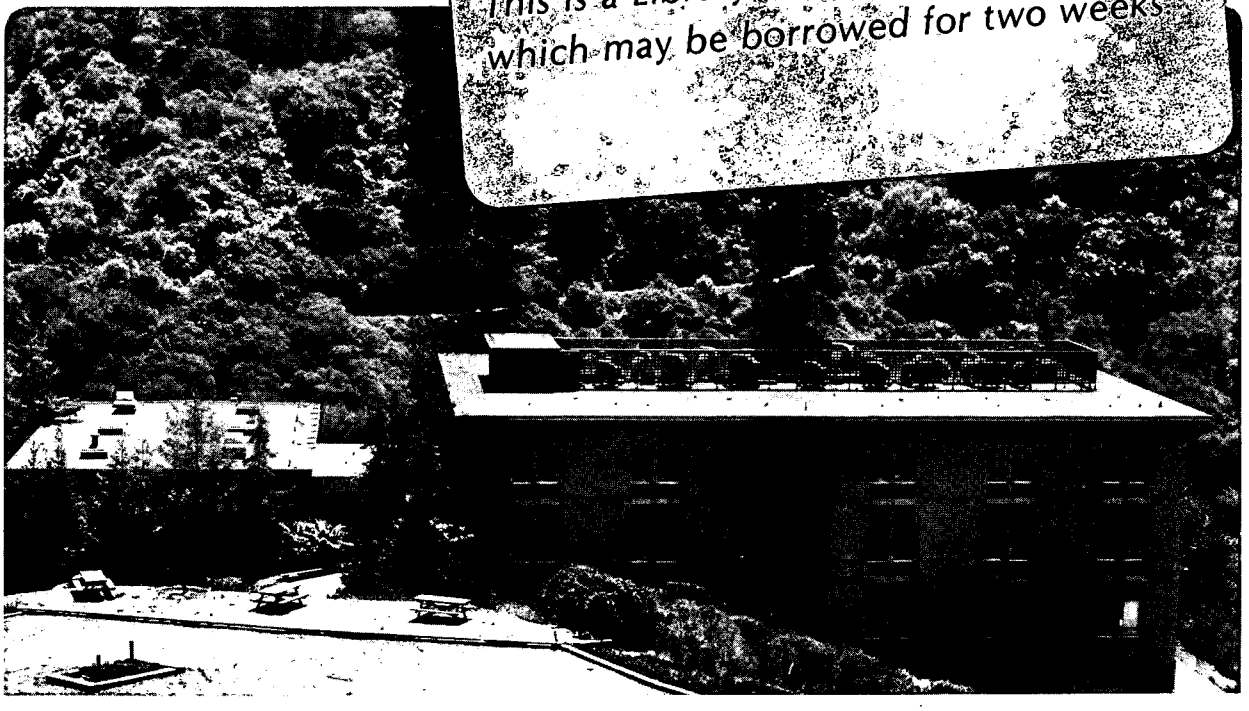

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Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

TRANSLATIONS AND STRUCTURE IN SYMMETRICAL TILT BODY-CENTERED-CUBIC GRAIN BOUNDARIES

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A simple geometrical method has been developed to calculate grain boundary translations that preserve first- and second-nearest neighbor coordination across the interface. These translations form interlocking polyhedral groups of atoms that define a mechanically stable boundary. Further individual atom relaxations can be easily recognized from the geometry of the atom arrangements. The description of boundary structure that results from this model is equivalent to a soft sphere description where a range of interatomic distances between the first and second-nearest neighbors exist at the grain boundary. A number of possible structures exist for each boundary; the relationship between these structures and the implications on grain boundary phenomena are discussed. A structural unit description results for particular sets of translations.

Introduction

The mechanical behavior of a grain boundary and the mechanics and kinetics of the movement of atomic species through and to the boundary can be predicted if a detailed atomic description of the boundary is available. The experimental problem in studying the atomic structure of grain boundaries are many, so experiments have been carried out on boundaries of well defined geometry. Diffraction[1] and high-resolution electron microscopy (HREM) techniques have been applied to this problem.[2] Most experiments were carried out in FCC crystal boundaries; only a near $\Sigma 41$ BCC boundary has been studied at atomic resolution by HREM.[3]

Alternatively, atomistic calculations were carried out which give the atom positions at the minimum energy configuration.[4] In particular, the calculations for BCC metals use interatomic potentials that are generated by fitting functional forms to experimental data. Typical of these is the Johnson potential for iron which shows a wide well between the first and second nearest neighbor distances. Under these conditions, in which the interactions with the first- and second-nearest neighbor are equally important, the body-centered cubic structure is stable.[5] These potentials are valid only when the coordination of the atoms in the calculation set is the same as that in the crystal. As is expected, the results of these calculations show that the boundary is composed of groups of atoms which are separated by distances between the first- and second-nearest neighbor distance and which retain the coordination of the crystal. That is, the atoms in the calculation volume obey the force law used. Although the principle of the atomistic calculations is simple, the implications of some of the characteristics of the calculation procedures (such as constant volume calculations and starting configuration) are still being reviewed.

The model presented here is a geometrical soft sphere model based on the assumption that the structure of the boundary in BCC materials is such that first- and second-nearest neighbor interatomic distances and coordination are preserved in the boundary region. The mathematical procedure to study boundary structure is developed in the next section. Examples of the structures of a Σ17 boundary are discussed in the third section and the implications on grain boundary phenomena are discussed in the last section.

Calculation Procedure

The procedure starts by calculating a grain boundary translation away from the coincidence relative position of the grains. This translation results in a group of atoms that defines a mechanically stable boundary. This is achieved in the following manner. The structure of a Σ17 [100]/(014) boundary is illustrated in Figure 1. Because of the mirror symmetry, the arrangement that an atom of the lower crystal sees in the upper crystal is the same as the arrangement that an atom in the upper crystal sees in the lower crystal. The full problem for a general boundary would require consideration of the relation between atoms of the lower crystal and the upper crystal after the translation. However, in the case of symmetrical tilt boundaries a simplification is possible. This arises because the displacements **t** and **–t** are symmetry related and thus the resulting structures are equivalent. The set of atoms used in the calculations is developed as follows. The atomic arrangement of the first layer of the upper crystal remains as is and the first layer of the lower crystal has been redrawn as seen by an atom of the upper crystal. Notice that the atoms that mark the period of the boundary coincide as in the CSL orientation. *The problem then has been reduced to the problem of positioning an atom sphere relative to a superposed arrangement of atoms.* A similar procedure has been used by Koiwa *et.al.*[6] The atoms numbered in Figure 1 are the atom positions used in the calculations. The problem of interest is then to place an atom in the surface composed of the atom positions numbered. *The position of the new atom defines a possible translation at the grain boundary. Thus, the position of the new atom is written as* (t_x, t_y, t_z). The coordinate frame is such that x is parallel to the tilt axis, y is normal to the tilt axis and contained in the boundary plane, and z is normal to the boundary plane and pointing towards the upper crystal. This implies that all possible translations have t_z negative.

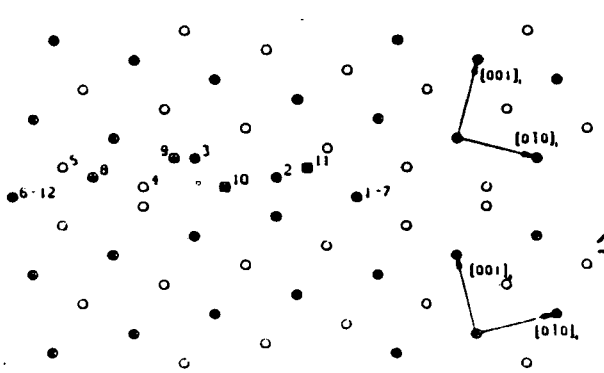

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Fig. 1 The Σ17 boundary at the CSL position and atoms used in the calculations

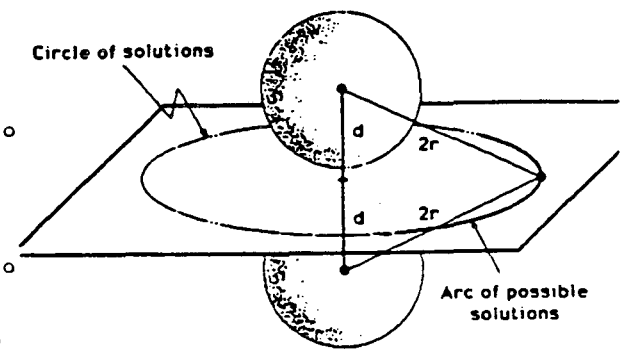

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Fig. 2 Solutions for a two sphere problem

If two atoms in the calculation surface are selected then a new sphere can be fitted within an arc of circle with radius r equal to the required interatomic distance. This situation is illustrated in Figure 2. The arc is part of a circle that lies on a plane normal to the vector that joins both spheres at the contact point. The circle of solutions is limited to an arc because of the presence of other layers of atom planes normal to the tilt axis. *Because of the mirror symmetry of the problem only translations with* $0 \leq t_z \leq \frac{r_{AB}}{2}$ *are studied.*

The first nearest-neighbor distance is indicated as D_1 and the second-nearest neighbor distance as D_2 and similarly for the corresponding radius. Consider first the FCC case where all atoms are equidistant. As it has been discussed above, the two-sphere problem has an infinite set of solutions (all contained in the arc of possible solutions). This implies that any given solution is mechanically unstable since there are other possible solutions in the immediate vicinity. A mechanically stable solution requires at least three contacts across the boundary per repeat unit of the boundary. A third atom is chosen and the center of a new sphere circumscribing simultaneously the other three is calculated. Of course, the new sphere can not overlap with any of the atom positions in the calculation surface. For each set of three atoms the coordinate frame is translated such that the origin coincides with the center of the circle in Fig. 2 and the y axis is along the vector that joins any two of the positions in the set of three. In this coordinate frame the new sphere center is given by

$$\begin{aligned} (t_z')^2 + (t_z')^2 + d^2 &= 4R_1^2 \\ (x_1' - t_z')^2 + (z_1' - t_z')^2 + (y_1')^2 &= 4R_1^2 \end{aligned} \tag{1}$$

where the prime indicates the new reference frame, and the third atom in the set, not shown in Fig. 2, is indicated by (x_1, y_1, z_1).

The solutions to Eqns. 1 are discussed briefly. The displacement in the primed x direction is given by

$$t_z' = \frac{m - 2z_1' t_z}{2x_1'} \tag{2}$$

where

$$m = (x_1')^2 + (y_1')^2 + (z_1')^2 - d^2 \tag{3}$$

The displacement in the primed z direction is given by the negative solution to the quadratic equation

$$\left[\frac{(z_1')^2}{(x_1')^2} + 1\right](t_z')^2 + \left[\frac{-mz_1'}{(x_1')^2}\right] t_z' + \left[\left(\frac{m}{2x_1'}\right)^2 + d^2 - 4R_1^2\right] = 0 \tag{4}$$

Special cases occurr of which the most important is when two of the atom positions coincide. Consider the set of atoms 1,2,7 in Fig. 1. Atoms 1 and 7 coincide but they are two different objects, and upon translation they exist as two different atom positions. However, from a mathematical point of view, we are back to the two-sphere problem. In order to solve this problem the displacement in the direction of the tilt axis is set arbitrarily to be equal to $r_{AB}/2$. This distance is indicated in the equations as m_z. With the origin of the coordinate system at the coinciding atoms, a set of equations similar to Eqns. 1 can be set-up. The solutions to these equations are

$$t_z' = \frac{p - t_y' y_1'}{z_1'} \tag{5}$$

where

$$p = \frac{1}{2}\left[(y_1')^2 + (z_1')^2 + (m_z - x_1')^2 - m_z^2\right] \tag{6}$$

and

$$\left[1 + \frac{(y_1')^2}{(z_1')^2}\right](t_z')^2 + \left[\frac{-2py_1'}{(z_1')^2}\right] t_z' + \left[m_z^2 + \frac{p^2}{(z_1')^2} - 4R_1^2\right] = 0 \tag{7}$$

This particular choice of the displacement in the direction of the tilt axis minimizes the excess volume and conserves the ordinary mirror symmetry.

The considerations of geometry and symmetry in the discussion presented here have reduced a problem with infinite solutions to a problem with analytical solutions. Up until now the discussion has been limited to the FCC case; the extension to the BCC case is straightforward and is discussed next.

Consider again the form of Equations 1. There are no restrictions on the values of the required distances which are given by the right hand side of the equations. In particular it is easy to require that the first-nearest neighbor distance be satisfied with two of the atoms in the set of three and that the second-nearest neighbor distance be satisfied with the remaining atom position.

$$\begin{aligned} (t_x')^2 + (t_z')^2 + d^2 &= 4R_1^2 \\ (x_1' - t_x')^2 + (z_1' - t_z')^2 + (y_1')^2 &= 4R_2^2 \end{aligned} \tag{8}$$

There are 8 cases for BCC calculations which are equivalent to Eqns. 8. These occur because for a given set of three atoms, there are $\binom{3}{2} = 3$ combinations of the three atoms taken R_1 at a time, and an equal number for R_2. In addition the new atom might be equidistant to all three in the set by either R_1 or R_2. These 8 cases are tabulated as programmed in Table 1 The solutions marked standard are the ones that have already been discussed in this section. All other solutions are just variations of these solutions and are discussed here. The solutions for case 5 are marked Standard‡ because the only modification necessary is to replace R_1 by R_2 in every equation. The solutions marked Modify† have for the regular cases

$$m = (x_1')^2 + (y_1')^2 + (z_1')^2 - d^2 + 4R_1^2 - 4R_2^2 \tag{9}$$

or for the coinciding cases

$$p = \frac{1}{2}\left[(y_1')^2 + (z_1')^2 + (m_x - x_1')^2 - m_x^2 + 4R_1^2 - 4R_2^2\right] \tag{10}$$

The solutions for the regular case are given as before by Eqns. 2 and 4, and the solutions for the coinciding case are given by Eqns. 5 and 7. For the solutions marked Modify§, m and p are given by Eqns. 9 and 10 except that R_1 changes to R_2 and viceversa. The solutions for the regular cases and coinciding case are given by Eqns. 2,4 and 5 and 7 with the same change in subscript. Finally, the coinciding solutions that are marked Not Possible in Table 1 can not occur because the atom positions 2 and 3 are always chosen as the coinciding positions by a subroutine ORDER that is described below. The new atom position then cannot be at two different distances from the same calculation surface position.

Table 1
BCC Analytical Solutions

Case	Distance to Positions			Comments on Solutions	
#	1	2	3	Regular	Coinciding
1	R_1	R_1	R_1	Standard	Standard
2	R_2	R_1	R_1	Modify†	Modify†
3	R_1	R_1	R_1	Modify†	Not Possible
4	R_1	R_2	R_1	Modify†	Not Possible
5	R_2	R_2	R_2	Standard‡	Standard‡
6	R_1	R_2	R_2	Modify§	Modify§
7	R_2	R_2	R_1	Modify§	Not possible
8	R_2	R_1	R_2	Modify§	Not possible

Comments on solutions are discussed in the text

The program developed for these calculations is described next. The first part of the program generates all the geometrical data from a few parameters that are particular for each boundary. The main DO loops of the program go through all possible sets of three atoms where 2 atoms belong to one crystal and the remaining to the other. On the basis of geometry some sets are discarded because a solution does not exist for that particular group. These are sets where two atoms are too far to possibly give a solution or where all three atoms belong to the same lattice. For each three atom set that can possibly give a solution the following subroutines are called.

Subroutine ORDER takes the three atom set and orders them such that atoms 2 and 3 are in the same layer and atom 2 is further from the boundary than 3. Under this order of the three atom set the solutions to the problem take the forms discussed in this section and summarized in Table 1. Subroutine NEWSPHERE produces the change of coordinates indicated in the text. The solutions to the problem are obtained in this prime coordinate frame and then backtransformed to the original coordinate system. Subroutine CHECK checks the solution obtained by NEWSPHERE so that no overlap with other atoms in the calculation surface occurs. In addition, the new solution is compared with the solutions already obtained since different atom sets can give the same solution. This indicates a particularly stable translation since additional redundant bonds across the boundary occur.

For each boundary translation the atom positions can be plotted as shown in Fig. 3a for a translation $t_x = .5$, $t_y = .59$, $t_z = -.64$ of the $\Sigma 17$ boundary shown in Fig. 1. From these atom positions, a very distorted picture of the boundary in terms of polyhedra appears. However, individual atom relaxations that would produce additional bonds of the required length are evident as shown in Fig. 3b. The structural unit description then is shown in Fig. 3c.

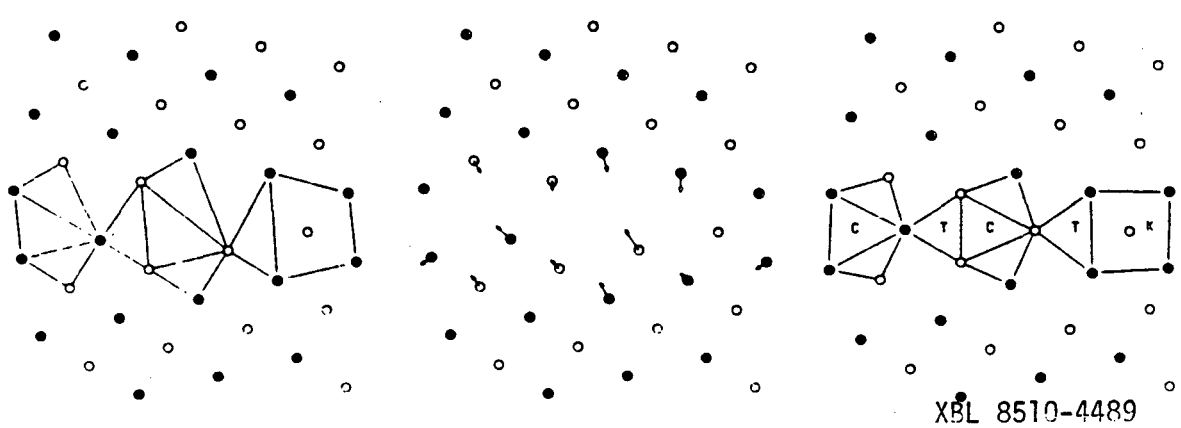

Figure 3. The relaxation procedure; (a) distorted structural units; (b) individual atom relaxations; (c) structural units

The graphical procedure of obtaining the individual atom relaxations is entirely justifiable since at present the atomistic calculations can not claim to be more accurate. In addition, the atomistic calculations give as result only one minima of the energy function, and in order to obtain other possible structures the calculations must be restarted from a different initial configuration. In the systematic procedure described here all possible minima of the energy function are generated at once with considerable savings of computational effort.

Example: The Structures of $\Sigma 17$

The result of the calculations described in the previous section is an interlocking group of 3 or 4 atoms. The set of all possible translations for the $\Sigma 17$ grain boundary is shown in Table 2 in order of increasing z component. Because of the symmetry of the atom calculation set about the half period, similar translations result from, for example, the sets 1,2,11

and 6,5,8. For a given case in Table 1 the translation that results from 1,2,11 corresponds to **t** while the translation obtained from 6,5,8, corresponds to **–t**. Only the positive translations are indicated in Table 2. *All numerical values of position are given in units of the lattice parameter.* Once the rigid-body translation is accomplished, further individual atom relaxations are evident that form additional groups of atoms that retain the interatomic distances of the crystal. Four typical structures are shown in Figures 3c and 4a-c. The symbols in the figures are chosen to indicate the AB stacking and the relative positions of the grains. The following notation is used to describe a given structure: C is a capped trigonal prism, K is a unit of BCC crystal, and T and O stand for a tetrahedron and an octahedron respectively. In all cases, the individual atom relaxations are large (>.25) only for 2 or 3 atoms per period. Thus, other than the distorted structural units shown at the grain boundary, additional tetrahedra, octahedra and BCC unit cells occur within 3 lattice parameters normal to the boundary.

TABLE 2
GB Translations for a BCC Σ=17 100 (014) Tilt Boundary

#	Translations in order of increasing z component (lattice parameter a=1.0)			New atom center at this position is distant to the atom centers indicated† by					
				.866a			a		
1	.4355	.7815	-.4819	11	2	-	10	-	-
2	.4242	.7653	-.4841	11	2	-	1	7	-
3	.3309	.6366	-.4850	11	2	1	-	-	-
4	.5000	.7099	-.4960	11	-	-	1	7	-
5	.5000	.5038	-.4961	11	7	1	-	-	-
6	.4922	.5108	-.4969	11	1	7	2	-	-
7	.1377	2.0616	-.4980	10 10	4 -	- -	3 9	- 3	- -
8	.0320	1.9327	-.5143	10	-	-	3	4	-
9	.3762	1.0257	-.5355	2	10	-	11	-	-
10	.1111	.6544	-.5562	2	1	7	11	-	-
11	.5000	.6566	-.5647	-	-	-	2	7	1
12	.2846	.8880	-.5712	2	-	-	11	10	-
13	.2136	.7884	-.5768	2	-	-	11	1	7
14	.5000	.3638	-.6063	1	7	-	11	-	-
15	.2909	.5395	-.6118	1	7	-	11	2	-
16	.3916	.6724	-.6281	-	-	-	11	2	1
17	.5000	.5878	-.6360	-	-	-	11	7	1

† Three atom sets are used in the calculations. If a fourth center is indicated, it is redundant. Only one set is shown. there are other sets of atoms that produce the same translation. These other sets are obvious from the symmetry of the grain boundary.

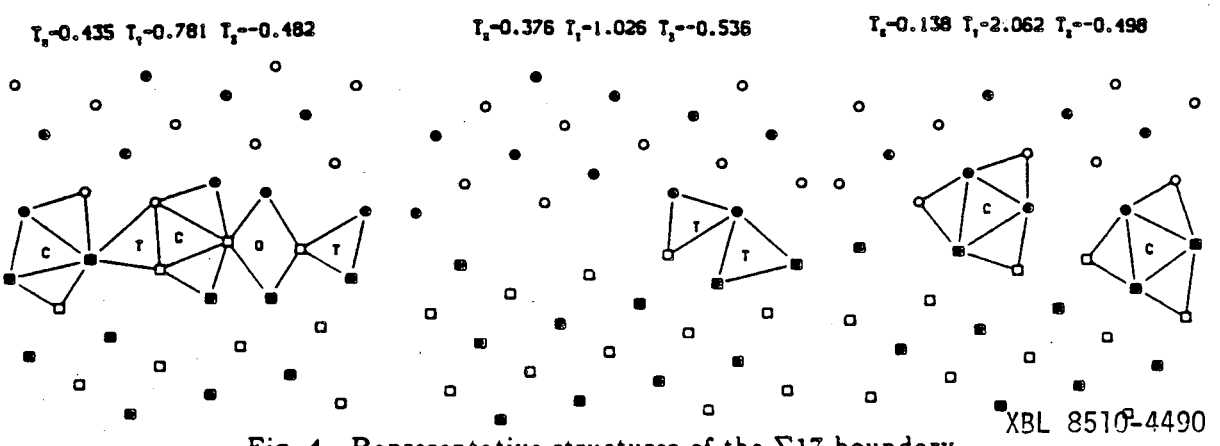

Fig. 4 Representative structures of the Σ17 boundary

Some translations produce a structure that can be described as a sequence of polyhedra that repeats with the period of the boundary. For example, the translations 5,7,14, (Fig. 3c) result in the sequence CTCTK while the translations 1,2,4,11,17 (Fig. 4a) result in the sequence CTCOT. These translations have a component parallel to the tilt axis close or equal to 0 or .5, as a result the ordinary mirror plane is conserved. Some translations form only a few structural units between the atoms in the set that originated that particular

translation. For example, the translations 3,9,10,12,13,15, and 16 (Fig. 4b) result in a group of two or three tetrahedra near the origin but it was impossible to relax the boundary further and create additional structural units. A particularly interesting set of translations is 7 and 8 (Fig. 4c). The y component of the translation moves the lower grain to one-half of the period of the boundary which is equal to 4.14. Because of the symmetry of the calculation set about the half-period (see Fig. 1), these translations are the result of a number of different atom sets and, in particular, translation 7 is the result of a Case 2 and a Case 7 (see Table 1). The boundary structure as shown in Figure 4c includes two capped trigonal prisms but the rest of the boundary cannot be relaxed to give additional structural units. Because of the symmetry of the calculation set the centers of the trigonal prisms are separated by half the period of the boundary. The translations that result in incomplete structural unit descriptions have a component parallel to the z axis which is different than .0 or .5. For these translations all symmetry elements are destroyed.

The criteria that have been established in order to obtain the most likely occuring boundary structure are to look for the structure with the highest coordination and with the minimum excess volume. The excess volume is linearly related to the z-component of the translation and thus to minimize the excess volume the lowest t_z is required. Of the two continuous structures indicated above, the one with the highest coordination is the structure CTCTK. This occurs because the atom positions are distorted in the structure CTCOT in such a way that the octahedral atoms inside crystals 1 and 2 have coordination 12 instead of coordination 14 (see Figs. 4a and 3c) . Thus, the most likely structure of the $\Sigma 17$ boundary is translation 5, illustrated in Figure 3c.

There are a number of grain boundaries that cluster in groups whose excess volume does not differ by more than 5%. One of these clusters is formed by the first 7 boundaries in Table 2. The translations of some of these boundaries are very close and thus the resulting structures are similar, for example, translations 5 and 6 and translations 1,2, and 4. Another important phenomenon that occurs for translations with similar z-component is the transformation between structures with different overall translation. These transformations occur by the addition or removal of a layer of atoms parallel to the boundary and the subsequent shift by d_p of the lower grain. For a symmetrical boundary with a planar density of coincidence sites equal to one, this represents the addition or removal of one atom per boundary period. It can be shown that the addition or removal of one layer parallel to the boundary plane is equivalent to an in-plane displacement. Thus, the difference between the in-plane components t_{x1}, t_{y1} and t_{x2}, t_{y2} is approximately equal to the crystallographic in-plane displacement corresponding to layer addition or removal. An example of such a transformation is the addition of one layer to translation 5 which transforms the most likely structure into the structure of translation 8. These transformations are extremely important in the description of grain boundary phenomena such as segregation. The change in structure of a grain boundary as the level of segregation increases occurs by transformations among the possible structures of a grain boundary. This point is discussed in detail in the next section. Some of the translations are exactly equal to a DSCL translation. For example, translation 14 is equal to $1/2[11\bar{1}]$ which is a crystal lattice translation and also a DSCL translation.

Continuity of Boundary Structure and Physical Processes

Each boundary in the sequence of [100] symmetrical tilt grain boundaries between $\Sigma 5$ and the perfect crystal was studied as the $\Sigma 17$ boundary described in the previous section. This sequence of boundaries can be described by a mixture of structural units of the $\Sigma 5$ boundary and the perfect crystal. The sequence of structural units for each boundary is shown in Table 2. The BCC tilt grain boundaries were also studied by Vitek, *et.al.* using molecular statics with the Johnson potential.[7] The structure of the boundaries calculated agree very well with the structures shown in this section. The atomic structure of $\Sigma 41$ agrees well

TABLE 2
Structural Unit Description of [100] Symmetrical Tilt Boundaries

Σ	*Angle*	*Plane*	*Structural Unit Sequence*
1	0	(001)	K,K,....
41	12.68	(019)	CTKKK-CTKKK,CTKKK-CTKKK,....
25	16.26	(017)	CTKK-CTKK,CTKK-CTKK,....
37	18.92	(016)	CTKKCTK,CTKKCTK,....
13	22.62	(015)	CTK-CTK,CTK-CTK,....
17	28.07	(014)	CTCTK,CTCTK,....
5	36.89	(013)	CT-CT,CT-CT,....

with the HREM experimental observations.

One of the more important aspects that results from this investigation is the existence of structures that are related by the addition or removal of one layer of atoms parallel to the boundary. Although the discussion that follows concentrates on the addition of a layer per period as would occur in grain boundary segregation, the problem of formation of substitutional point defects at the boundary can be described by the inverse phenomenon of removal of one layer per period of the boundary. Segregation occurs then simply by adding one atom per boundary period. The sequence of structural units for a period without segregation will be indicated by a U, and the sequence of units in a period where segregation has occured by S. The U periods and S periods have the same excess volume. Thus the two structures have different in-plane translations. This implies that at the region where an U unit joins a S unit, a partial grain boundary dislocation with Burgers vector equal to the difference in translations exists. Since this defect has an energy associated with it, segregation would tend to occur in such a way that the number of these defects is minimized. Under non-equilibrium conditions segregation occurs randomly along the boundary as the segregating atom species arrive at the boundary plane. Upon annealing, U units and S units will cluster to minimize the energy associated with the partial grain boundary dislocations. This implies that changes in concentration along the boundary plane should occur, and that the clusters of S units are preferential sites for the heterogeneous nucleation of second phases or for crack nucleation due to fragility at the boundary plane induced by the segregating species. Variations of the concentration of a segregating species along the boundary plane have been reported.[8]

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This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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