COINCIDENCE LATTICE MODEL FOR THE STRUCTURE AND
ENERGY OF GRAIN BOUNDARIES

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ABSTRACT

The Coincidence Site Lattice (CSL) model of grain boundaries is developed on a simple physical basis. We propose that, to a good approximation, the construction of a boundary can be described in terms of three basic steps: 1) a rigid body joining of two perfect crystals along the boundary plane (Step I); 2) a primary relaxation (Step II) consisting of relaxations in the boundary centered on O-Lattice elements which act to improve lattice matching in these regions; and 3) a possible secondary relaxation (Step III) which produces the final structure composed of patches of a low Σ boundary and secondary grain boundary dislocations. The energy after Step I is obtained by summing pairwise interactions across the boundary and is found to be relatively low for a number of low Σ boundaries and to approach a larger constant value for all large Σ boundaries. The energy decrease due to Step II varies monotonically with crystal misorientation according to a Read-Shockley function, and the energy decrease associated with Step III produces cusps in the energy versus misorientation curve at misorientations corresponding to low Σ boundaries. The model appears to be consistent with our present knowledge of boundary structure and energy, and its general applicability is discussed.

1. INTRODUCTION

The purely geometrical model of grain boundary structure based on the Coincidence Site Lattice (CSL) [1] has been widely used in efforts to interpret the structure and energy of large angle grain boundaries [1-4]. In this approach, it is assumed that a grain boundary may be of relatively low energy when the two adjoining crystals form a relatively dense CSL. When this is the case, and the crystal misorientation deviates from the high density CSL misorientation, it is proposed that a network of secondary grain boundary dislocations (SGBDs) may be formed which compensates for the deviation and produces a structure consisting of the SGBD network embedded in the low energy interface associated with the high density CSL.

This model has met with considerable success in the interpretation of experimental results. For example, evidence for the existence of cusps in boundary energy versus crystal misorientation plots at high density CSL misorientations has been obtained [5,6], and numerous SGBD networks have been observed [7] under expected conditions. Computer calculations using the method of molecular statics have also supported various aspects of the model; in this work, an assemblage of atoms constituting the bicrystal is set up, and it is assumed that the atoms interact via a central force pairwise potential. The boundary structure of minimum energy is then calculated by computer methods. Such calculations [8-11] have shown that high density CSL boundaries are often of relatively low energy, and that SGBDs indeed form at intermediate misorientations. Much of this work has been reviewed recently in [12].

The purpose of the present paper is to develop the CSL model on a simple physical basis. As will be seen, we base our approach on relatively simple concepts and employ various approximations. The results are

therefore not suited to the precise calculation of specific structures and energies. Nevertheless, the model provides a conceptual framework for understanding the physical basis of boundary structure and energy.

2. BASIC DESCRIPTION OF MODEL

Any grain boundary can be constructed by joining two rigid crystals along the boundary plane and then allowing the configuration to relax. We, therefore, visualize the construction of a boundary to consist of the following three steps:

Rigid body joining (Step I): Lattices 1 and 2 are joined together rigidly along a macroscopically flat interface to form the grain boundary. In this process all atoms in Lattices 1 and 2 are held rigidly in their perfect lattice positions, and Lattice 2 is translated with respect to Lattice 1 so that minimum energy is achieved. In general, Lattice 2 is misoriented with respect to Lattice 1 by an angle θ to form a CSL. At the end of this step, as demonstrated in Section 3, we expect the boundary energy, E_R , of both twist and tilt boundaries, to depend upon Σ (the reciprocal of the fraction of lattice sites in coincidence) at relatively low values of Σ and to be independent of Σ at large Σ values.

Primary relaxation (Step II): in this step primary relaxations occur in regions of the boundary centered on the elements in the boundary of an appropriately chosen O-Lattice as described by Bollmann [1]. Each such element (i.e., "O-element") serves as an origin for a relaxation in its vicinity which acts to improve local lattice matching across the boundary. The motivation for this relaxation is, therefore, the reduction in energy which accompanies this improved matching. The spacing of the O-elements

varies monotonically with the crystal misorientation angle θ and, hence, the scale on which these relaxations occurs depends continuously on θ . We, therefore, expect the change in boundary energy in this step, E_p , to vary continuously with θ .

Secondary relaxation (Step III): finally, we imagine that secondary relaxations occur in high Σ boundaries having misorientations differing from those of certain nearby low Σ misorientations to produce structures consisting of SGBDs and patches of the low Σ boundary. As shown in Section 5, we expect the change in energy due to this step, i.e., E_S , to vary with both the Σ value of the nearby low energy CSL misorientation and $\Delta\theta$, the deviation of the crystal misorientation from that of the nearby low energy CSL misorientation.

The total boundary energy, E , is, therefore, given by

$$E = E_R + E_p + E_S \quad (1)$$

Equation (1) is the basic equation of our CSL model and expresses the hypothesis that, to a reasonably good approximation, the energy can be broken down into the individual terms indicated. We now consider each of these terms in detail.

3. RIGID BODY JOINING (STEP I)

In order to establish our model we work with [001] twist and symmetric tilt boundaries. These boundaries are relatively simple and convenient for this purpose.

[001] twist boundaries: Step I can be accomplished by starting with a large, single crystal lattice block with {100} faces having energy E_0 . This may be divided in half along a (001) plane into two blocks (Lattices 1 and 2) which are then separated (without rotation) to infinity requiring energy ΔE_1 . The rigid boundary is then produced by rotating Lattice 2 with respect to Lattice 1 by the angle θ around [001] at the large separation and rejoining the blocks to form the bicrystal. If the energy change (per unit area of grain boundary) involved in this operation is ΔE_2 , then the rigid boundary energy is

$$E_R = (E_0 + \Delta E_1 + \Delta E_2) - E_0 = \Delta E_1 + \Delta E_2, \quad (2)$$

where ΔE_1 is constant for all [001] twist boundaries; the energy ΔE_2 is taken as the sum of all the central force pairwise interactions between the ions of Lattices 1 and 2 (per unit area of grain boundary) as the two crystals are brought together so that (to within the additive constant, ΔE_1)

$$E_R = \sum_{\text{pairs}} v(\vec{r}), \quad (3)$$

where $v(\vec{r})$ is the pairwise potential, and the sum is over all ion pairs separated by the boundary

We now show that the sum in Eq. (3) can be evaluated in a particularly convenient way within the framework of the DSC-Lattice [1,2]. If it is imagined at first that both lattices are positioned so that they occupy

sites on the CSL as illustrated in Fig. 1(a), then it may be shown, as demonstrated in the Appendix, that the vectors connecting the atoms in the (001) plane of Lattice 1 in the CSL unit cell shown (of which there are Σ) with all of the atoms in the (001) plane of Lattice 2 in the same plane of the CSL are given by all vectors of the DSC-Lattice shown in Fig. 1(b). Therefore, in the final relaxed bicrystal configuration (where Lattice 2 may occupy some off-CSL translational position with respect to Lattice 1) the interaction energy between the p^{th} (001) plane of Lattice 1 with the 1^{th} (001) plane of Lattice 2 may be written (per unit area of boundary) as the sum

$$e_R(p,1) = \frac{1}{a^2 \Sigma} \sum_{R_{i,j}} v(\vec{R}_{i,j} + \vec{t}_{p,1}) \quad , \quad (4)$$

where $\vec{t}_{p,1}$ is a vector connecting an atom in the p^{th} plane of Lattice 1 with one in the 1^{th} plane of Lattice 2; $\vec{R}_{i,j}$ is a vector in the DSC-Lattice frame (Fig. 1); and a is the nearest-neighbor lattice spacing (Fig. 1). The sum is taken over all points (i,j) of the DSC-Lattice including the origin in Fig. 1(b). The final total rigid boundary energy is then obtained by summing over all planes across the boundary; i.e.,

$$E_R = \sum_p \sum_l e_R(p,l) \quad (5)$$

We have calculated the energy E_R for a number of [001] twist boundaries with different Σ values in the FCC and BCC structures. For the FCC case a pairwise potential of the Lennard-Jones type (fit to krypton) was used, whereas, for the BCC case the Johnson potential [13] (fit to α -iron) was used. For each boundary Lattice 2 was translated with respect to Lattice 1 by both in-boundary and out-of-boundary translations to find

the final structure of minimum energy. The results are shown in Fig. 2 where it is seen that the energies of the relatively low Σ^* (high density CSL) boundaries are found to be generally lower than those of the high Σ boundaries. Also, the energies of the higher Σ boundaries approach an asymptotic value at very large Σ values. The energies appear to increase in an approximately monotonic manner for these particular boundaries. However, despite extensive efforts, we were not able to demonstrate this monotonic behavior by any analytical method, and we must therefore conclude that it may not be general. Similar results have been obtained previously by Bristowe and Crocker [14] who calculated the rigid body energies of (001) twist boundaries using pairwise potentials for copper and nickel. Their results, normalized to values of $E_R(\Sigma \rightarrow \infty)$ estimated from the present work, are plotted in Fig. 3.

The asymptotic behavior at large Σ values found by the computer calculations may be verified by an analytical procedure. The geometry of the problem of summing the energy for two planes across the boundary is illustrated in Fig. 4. The planar density of DSC-Lattice points contributing to the sum of Eq. (4) is given by Σ/a^2 . Therefore, when Σ becomes very large the density of summing points in Fig. 1(b) becomes exceedingly high and can be taken to be constant over the 1th plane. The interaction energy, therefore, becomes independent of the horizontal position of the 1th plane, and the summation in Eq. (4) can be replaced by an integral of

* In the present work "low" Σ boundaries are taken to be boundaries with Σ less than about 50. As seen in Fig. 5, these boundaries generally have energies significantly lower than the asymptotic value which is approached as $\Sigma \rightarrow \infty$. The remaining boundaries are considered to be "high" Σ boundaries.

the form

$$e_R(p,1) = \frac{1}{\Sigma a^2} \int_0^\infty v(\sqrt{s^2 + \rho^2}) \cdot 2\pi\rho d\rho \cdot \left(\frac{\Sigma}{a^2}\right), \quad (6)$$

where s is the constant projection of t on the boundary normal, and ρ is a radius vector in the 1th plane (Fig. 4). The right hand side of Eq. (6) is seen to be independent of Σ , since the effect on $e_R(p,1)$ of varying s does not have any Σ dependence under these conditions. Since this result is true for any $p,1$ pair of planes, it must also be true for E_R given by Eq. (5).

[001] symmetric tilt boundaries: generally similar results are obtained for the tilt boundaries. The pairwise sums across the boundary can again be represented within the framework of the DSC-Lattice, but here the problem is somewhat more complicated, since complete coverage of the DSC-Lattice is not achieved (see the Appendix). Also, ΔE_1 in Eq. (2) must be evaluated for each Σ .

Values of E_R calculated for a series of symmetric tilt boundaries in the FCC and BCC structures using the same Lennard-Jones and Johnson potentials as previously, are shown in Fig. 5. Again, we find that the energies of relatively low Σ boundaries are lower than those of the high Σ boundaries and that the energies of the high Σ boundaries approach an asymptote.

We therefore find that the calculated energies of all of the rigid body boundaries after Step I increased in an approximately monotonic way with Σ (Figs. 2, 3 and 5) even though we cannot conclude that this monotonic behavior is true in general. The relatively low energies of the low Σ boundaries after the rigid body joining step may be interpreted as due to

a difference between a pairwise sum (e.g., Eq. (4)) for the low Σ boundaries and an integral (e.g., Eq. (6)) for the high Σ boundaries. At low Σ the summation process in the DSC-Lattice frame becomes "grainy", and it is possible to fit Lattices 1 and 2 together in their minimum energy configuration in special ways which often lead to relatively low energies. At high Σ this is no longer possible, and, as we have seen, the energy becomes independent of Σ .

4. PRIMARY RELAXATION (STEP II)

The particular O-Lattice which should act as the framework for the primary relaxation should correspond to the transformation between Lattices 1 and 2 which relates nearest-neighbors of Lattices 1 and 2 in the vicinity of each O-element. As Bollmann has pointed out [1], this O-Lattice should be the most relevant physically, since the ensuing primary relaxations should then act to improve lattice matching in the vicinity of the O-elements. For [001] twist and tilt boundaries this O-Lattice corresponds to a simple rotational transformation, $A(\theta)$, between Lattices 1 and 2. As is well known [1], the vectors, $\vec{X}^{(0)}$, of this O-Lattice are given by

$$\vec{X}^{(0)} = \{I - A^{-1}\}^{-1} \vec{X}^{(L1)} \quad (7)$$

where $\vec{X}^{(L1)}$ are the vectors of Lattice 1.

[001] twist boundaries: for [001] twist boundaries in the FCC structure this O-Lattice projects on the boundary as a square array of points with mesh spacing:

$$|\vec{X}^{(0)}| = \frac{a_o}{\sqrt{2} \cdot 2 \sin(\theta/2)} \quad (8)$$

where a_0 = lattice parameter. Since the 0-Lattice spacing varies continuously with θ we also expect the primary relaxation and its accompanying energy change, E_p , to vary continuously with θ . As is well known [1], at small angles the primary relaxation at the end of Step II produces a boundary which to a good approximation can be considered as made up of discrete and uniformly spaced lattice screw dislocations. The boundary energy in this angular range is mainly due to the elastic energy in Lattices 1 and 2 of the dislocation array which, as shown by Read and Shockley [15], depends upon θ according to $-Ab\theta \ln(\theta/\theta_c)$, where A and θ_c are constants, and b = magnitude of Burgers vector. At higher angles the dislocation cores approach one another and eventually impinge, and the energy can then no longer be calculated from simple elasticity theory. In order to cope with this situation in the present model, we make the reasonable approximation that the total energies of all of the high Σ boundaries after the primary relaxation has occurred are given by:

$$E_R + E_P = \begin{cases} -Ab\theta \ln\left(\frac{\theta}{\theta_c}\right) + \frac{\theta E_c}{b} & \dots (\theta < \theta_c) \\ \frac{\theta_c E_c}{b} & \dots (\theta > \theta_c) \end{cases} \quad (9a)$$

where θ_c = critical angle at which the dislocation cores just impinge, and E_c = core energy of the dislocations per unit length. This corresponds to a model consisting of discrete dislocation cores at angles below θ_c , where the energy is given by the sum of the elastic energy of the dislocations [first term in Eq. (9a)] and their core energy (second term). At $\theta = \theta_c$ the cores impinge, and from then on the boundary energy is simply assumed to remain constant at the value $\theta_c E_c / b$. A reasonable value for

θ_c is $\theta_c = \pi/9$.

Now, if, for example, we replot E_R as a function of θ for the twist boundary with the Lennard-Jones potential presented previously in Fig. 2 (with the convention that $E_R(1) = 0$), we obtain the plot shown in Fig. 6. Therefore, $E_p(\theta)$ must be of the form

$$E_p(\theta) = \begin{cases} -E_R(\Sigma=\infty) - Ab\theta \ln\left(\frac{\theta}{\theta_c}\right) + \frac{\theta E_c}{b} & \dots (\theta < \theta_c) \quad (10a) \\ -E_R(\Sigma=\infty) + \frac{\theta_c E_c}{b} & \dots (\theta > \theta_c) \quad (10b) \end{cases}$$

which is plotted schematically in Fig. 7. The energies of all boundaries at this stage are therefore obtained by adding E_R and E_p , and these are shown in Fig. 8.

[001] symmetric tilt boundaries: the analysis for the series of [001] symmetric tilt boundaries with $0^\circ < \theta < 45^\circ$ is similar in many respects to the above treatment for twist boundaries. The O-Lattices are, of course, the same as for the twist boundaries, but now the boundary plane runs parallel to the [001] rotation axis and, therefore, the O-elements in the boundary consist of "O-lines" (running parallel to [001]) rather than "O-points". In the range $0^\circ \leq \theta \leq 45^\circ$ the spacing between O-lines in the boundary in a FCC structure is given by

$$l = \sqrt{2} \cdot |\vec{X}^{(0)}| = \frac{a_u}{2\sin(\theta/2)} \quad (11)$$

The expected primary relaxation, therefore, consists of rotations of both Lattice 1 and Lattice 2 around each O-line in a direction to decrease θ locally in the Wigner-Seitz cell containing each O-line. We again expect

$E_p(\theta)$ to obey an equation of the form of Eq. (10), and if we combine this result with results of the type illustrated in Fig. 5 we obtain plots of $[E_R + E_p]$ versus θ for tilt boundaries which qualitatively resemble the plot shown in Fig. 8 for the twist boundaries.

5. SECONDARY RELAXATION (STEP III)

At this stage the boundary energies appear as in Fig. 8. Many high Σ boundaries may now reduce their energy further by undergoing a secondary relaxation as described in Section 2. This decrease in energy may be evaluated for large Σ boundaries possessing misorientations close to those of a low Σ boundary for appropriate choices of the SGBD arrays which are produced. To a good approximation, the total energy of a boundary consisting of an array of SGBDs embedded in a low Σ interface of energy $E(0)$ may be written in the form

$$E(\Delta\theta) = E(0) - \Lambda b \Delta\theta \ln \left(\frac{\Delta\theta}{\Delta\theta_c} \right) + \Lambda \theta \frac{E_c}{b} \quad (12)$$

when $\Delta\theta$ is small and the SGBD spacing is correspondingly large. The second and third terms in Eq. (12) represent the elastic energy and core energy of the SGBD array. The latter term may include a significant contribution from the step in the boundary plane which may be associated with each SGBD [16]. A set of typical curves obeying Eq. (12) is shown schematically in Fig. 9. The cusp for each curve is located at the energy of each low Σ boundary, i.e., $E(0)$, and the changes in energy due to the secondary relaxation, E_S , are then the differences between these curves and the values of $E_R + E_p$ which were transferred from Fig. 8. The result is a significant decrease in energy for many of these boundaries (see example

in Fig. 9) and the appearance of cusps in the $E(\theta)$ curve at the low Σ misorientations.

We are now interested in the shapes of these curves further from the cusps and how the various curves for the choices of the possible SGBDs join up to produce a single $E(\theta)$ curve corresponding to the boundary structures of minimum energy at all misorientations. Clearly, the equilibrium boundary structures at all misorientations will correspond to the lowest envelope of all the possible curves. In view of this, it may be concluded that some of the relatively low Σ boundaries in Fig. 9 may themselves undergo secondary relaxations and decrease their energies further by developing grids of SGBDs if other curves fall below them.

It is impossible to proceed further without specific information about the detailed structures and energies of the various possible boundaries as $\Delta\theta$ increases and the SGBD spacing decreases. This can only be obtained from atomistic calculations.

Fortunately, Sutton and Vitek [9-11] have carried out such calculations recently for several series of boundaries by the method of computer simulation using a pairwise potential. These important calculations have clarified further details of the secondary relaxation, and we therefore discuss some of their results in the next section and point out how they can be used to extend the present model. Briefly, their work indicates that all boundaries at all misorientations can be realistically described in terms of the CSL model. In addition, it may be concluded that certain of the low Σ boundaries at the cusps in Fig. 9 are indeed minimum energy structures and remain fixed in structure and energy, i.e., they do not undergo a secondary relaxation. These are termed "favored" boundaries. The energies of all other boundaries decrease to a greater or lesser extent as the secondary

relaxations occur and SGBDs appear. Relatively major cusps in the $E(\theta)$ curve form at the favored boundary misorientations and generally weaker cusps appear at the misorientations of unfavored boundaries corresponding to relatively low Σ values.

6. FURTHER ASPECTS OF MODEL AND DISCUSSION OF RESULTS IN LITERATURE

Rigid body joining step: the set of energy differences between boundaries of different Σ which is established at the end of the rigid body joining step is the primary basis for the existence of the favored boundaries and their associated cusps in the present model. As already seen, the boundary energies at the end of this stage increased with Σ almost monotonically for the particular cases calculated in the present work (Figs. 2, 3 and 5). However, it is recognized that this result may not be true in general. In any event, the final relaxed energies of the low Σ boundaries responsible for producing significant cusps are not expected to scale with Σ in any simple way. This is because the final energy of any favored boundary depends upon both Σ and θ in the present model as a result of the contribution of the rigid body energy and the energy change due to the primary relaxation. Also, the energies of the relatively low Σ unfavored boundaries depend upon their misorientations relative to those of the nearby favored boundaries.

It appears likely that the major components of any final rigid body translation of Crystal 2 with respect to Crystal 1 are established in the rigid body joining step in the present model. Any rigid body displacements

in Steps II and III are almost certainly small and do not appear explicitly in our treatment. In this respect it is noted that Bristowe and Crocker [14] found that there were three basic types of final rigid body translations which led to stable [001] twist boundaries in copper and nickel. These translations corresponded to positioning Lattice 2 (in projection):

(1) on the origin of a DSL-Lattice cell; (2) on the center of a DSL-Lattice cell; and (3) on the center of one edge of a DSL-Lattice cell. If we consider the total interaction to be the sum of all the interactions between planes it is readily seen from Fig. 1 for the rigid body joining step that these three translational positions are the only positions which possess the necessary symmetry so that the total force exerted by Lattice 1 on Lattice 2 in the plane of the boundary is zero. (Other arrangements in which the forces would oscillate from plane to plane but sum to zero seem impossible, since the force between two planes becomes weaker as the separation between planes increases.)

Primary relaxation step: there is extensive experimental and computational evidence in support of the O-Lattice and primary relaxations described in Section 4. Electron microscope observations [17] of small angle [001] twist boundaries ($0^\circ < \theta \lesssim 15^\circ$) in gold have clearly revealed the existence of square networks of lattice screw dislocations where each network mesh opening is centered on one of the O-elements of the O-Lattice described in Section 4 which are distributed in the boundary at an average spacing given by Eq. (8). In our model the total relaxation should consist of the sum of the primary and secondary relaxations. The effect of the secondary relaxation is relatively small at small angles and, therefore, the existence of these dislocations is direct evidence for a primary relaxation in which Lattices 1 and 2 rotate with respect to one another around each O-element

by the angle $-\theta$ to restore perfect lattice matching across each local region. At larger angles the O-elements become closer together, and finally it is no longer possible to produce square patches of perfect lattice by means of the primary relaxation. Nevertheless, a relaxation consisting of a rotation around each O-point in a direction to reduce the rotational misorientation across the boundary still occurs. This conclusion has been supported by direct imaging of the displacement field of the primary relaxation in large angle [001] twist boundaries in gold in the electron microscope [17] and by the observation of relatively strong "O-reflections" in the electron and X-ray diffraction patterns from these same boundaries due to the periodic displacement field of the primary relaxation [18,19].

The existence of this type of primary relaxation is also evident in the structure of [001] twist boundaries in FCC metals as revealed by computer simulation. Bristowe and Crocker [14] have calculated the fully relaxed structures of a series of large angle [001] twist boundaries [i.e., $\Sigma=5(36.9^\circ)$, $\Sigma=13(22.6^\circ)$, $\Sigma=17(28.1^\circ)$ and $\Sigma=25(16.3^\circ)$] in copper and nickel, and these structures are reproduced in Fig. 10 along with the vector components in the boundary plane (magnified 5 times) of the atomic displacements associated with the total relaxation. It may be seen directly that a strong relaxation occurs in each Wigner-Seitz cell centered on each O-element which can be most generally described as a rotation of Lattice 2 with respect to Lattice 1 around the O-element in a direction to reduce θ locally. The relaxation displacements are almost exactly tangential around the O-elements well within the cells but become less so near the cell boundaries. Nevertheless, the tangential components are always in the $-\theta$ direction. Furthermore, the displacements are zero for

atoms directly on the O-elements such as in Fig. 10(b) and at the A's in Figs. 10(a), (c) and (d). A further example of this type of primary relaxation in a [001] ($\Sigma=5$) twist boundary in the BCC metal tungsten calculated in [20] is shown in Fig. 11. In this case the interatomic potential is particularly "hard", and the rotations around the O-elements are considerably larger than the previous examples and therefore may be seen directly. All these primary relaxations at the larger twist angle are qualitatively similar to those which occur at small angles, and the primary relaxation, therefore, exhibits essentially continuous behavior as θ increases from zero to the maximum angle of 45° .

There is also evidence for such a primary relaxation over the full range of θ for [001] tilt boundaries. Electron microscope observations [21] of small angle [001] tilt boundaries ($0^\circ < \theta \lesssim 13^\circ$) in gold have revealed the expected primary relaxations around the O-lines, and the result is a family of discrete lattice edge dislocations at an average spacing given by Eq. (11).^{*} Evidence for the relaxation at larger angles has come from both X-ray diffraction and electron microscopy diffraction and imaging studies. Diffraction patterns taken at normal incidence to the grain boundary plane in gold reveal O-reflection satellite spots distributed around the lattice reflections at spacings which are reciprocals of the O-line spacings in the boundaries [23]. In other experiments with gold [24] it has been shown that the O-reflections have relrods associated with them which run in a direction perpendicular to the grain boundary plane. The length of these relrods should be reciprocally related to the "thickness" of the boundary, i.e., the

* The dislocation structure of these boundaries in metals of relatively low stacking fault energy is somewhat complicated by a tendency of the dislocations to become serrated in an effort to dissociate on $\{111\}$ planes [22]. However, this complication does not greatly affect the main aspects of the present analysis.

depth to which its displacement field penetrates the adjoining crystals. The experimental results show that the "thickness" of the boundary measured in this way is directly proportional to the O-line spacing in the boundary which is just the result to be expected if primary relaxations occur around each O-line. In still further work, Cosandey and Bauer [25] have used lattice imaging methods to reveal directly the displacement field of the primary relaxation in [001] tilt boundaries in gold and find that a primary relaxation occurs around the O-lines regardless of the angle of misorientation and inclination of the boundary plane. Finally, we point out that the relaxations around the O-lines can be seen directly in boundary structures obtained by computer simulation. Figure 12 shows the atom displacement field in a [001] $\Sigma=5$ ($\theta=36.9^\circ$) tilt boundary in BCC iron which we have calculated using the Johnson interatomic potential. It is evident that atoms in the core region have relaxed mainly in a direction to reduce the tilt misorientation in the vicinity of each O-line as expected.

It is interesting to note that the relaxations around the O-elements, as described in the present model, appear to have further physical significance for other relaxations in the boundary in response to perturbations. As an example, in other work [20] we have used molecular statics to calculate the atomic displacements around vacancies in a number of [001] twist boundaries. It has been found that a major component of the relaxation again corresponds to tangential displacements of nearby atoms around O-elements. Figure 13 shows the atomic displacement field in the [001] $\Sigma=5$ twist boundary in tungsten already shown in Fig. 11 which was produced by inserting a vacancy at the atomic site in the boundary indicated by the circle. The strong tangential components of the relaxations around the O-elements are evident.

Secondary relaxation step: as mentioned in the previous section, Sutton and Vitek [9-11] have recently carried out detailed atomistic calculations for several series of boundaries which reveal further details of the boundary structure and allow us to extend the present model for the secondary relaxation. They find that the cores of certain relatively low Σ boundaries in each of these series are actually comprised of a uniform array of a single type of "structural unit". (A structural unit is defined as a small group of atoms arranged in a characteristic configuration.) These boundaries, which are termed "favored" boundaries, are, therefore, extremely uniform in structure and consist of a contiguous sequence of primary (lattice) dislocations whose long range elastic stress fields cancel. Therefore, no significant stress field can be detected near them in the adjoining lattices by computer simulation. All other boundaries which possess misorientations which are intermediate between those of the favored boundaries possess structures which are simply mixtures of the units making up the two nearest favored boundaries. The structures of these intermediate (or "unfavored" boundaries) are, therefore, derived from a simple rule of mixing of the units of the nearby favored boundaries. Furthermore, the description in terms of mixtures of structural units corresponds directly to one in terms of SGBDs. In the case of unfavored boundaries which are intermediate between two favored boundaries consisting of all A type units and all B type units respectively, the structure of boundaries near the favored A type boundary consists of B units embedded in an array of a larger number of A units. In such cases, each B unit is the core of a SGBD having a Burgers vector belonging to the DSC-Lattice of the favored A type boundary. For misorientations near that of the favored B type boundary the structure consists of A units embedded in an array of a

larger number of B units, and an A unit acts as the core of a SGBD having a Burgers vector belonging to the DSC-Lattice of the favored B type boundary. At some intermediate misorientation the numbers of A and B units are equal. The cores of these SGBDs are therefore quite narrow, i.e., localized, and, very importantly, they retain their identity at small spacings. These results therefore provide strong support for the CSL model at all misorientations.

In view of these results we may express the energy of any unfavored boundary as the sum of the self-energies of the A and B units which are present plus the sum of all the interaction energies between them. Therefore,

$$E = n_A e_A + n_B e_B + E'_{AB} + E''_{AB} \quad , \quad (13)$$

where n_A and n_B are the numbers of A and B units, e_A and e_B are the self-energies of the "perfect" individual units in the favored boundaries, E'_{AB} is the interaction energy between A and B units, and E''_{AB} is the elastic energy in the adjoining lattices associated with the presence of the units. The E'_{AB} term arises because the A and B units in the unfavored boundaries are often significantly distorted relative to their perfect structures.

It is impossible to predict the exact form of E in Eq. (13) as a function of θ in any simple way, since a detailed calculation of the core energy would be required in each case. Nevertheless, because of the simple rule of mixing units, it is anticipated that the sum of the energies of the first three terms will normally vary in a simple continuous manner with θ in the angular range between the favored boundaries as illustrated, for example, by the dashed line in Fig. 14. Next, the elastic interaction energy, E''_{AB} , should be given by the elastic energy of the SGBD array. For

the special cases where the A or B units are uniformly spaced, the corresponding SGBDs are uniformly spaced, and this energy should take the form

$$E'_{AB} = -Ab\Delta\theta \ln\left(\frac{\Delta\theta}{\Delta\theta_c}\right), \quad (14)$$

where b = vector of the appropriate DSC-Lattice corresponding to the θ_B or θ_A misorientation. The addition of this term to the energy produces cusps at the favored boundary misorientations as shown schematically by the dotted curves in Fig. 14. Each dotted curve has its origin at θ_A or θ_B , and they meet at the point M where equal numbers of A and B units are present.

The dotted curves in Fig. 14 hold only for the cases where the SGBDs are uniformly distributed. It may be shown [26] that this condition is achieved only at misorientations corresponding to relatively low Σ values. At small deviations from these special misorientations topological constraints require that the A or B units be distributed non-uniformly. However, such a non-uniform distribution of A or B units can be represented by a further array of SGBDs embedded in the nearby boundary consisting of the uniform distribution of A or B units [26]. Furthermore, the Burgers vectors of this SGBD array are vectors of the DSC-Lattice corresponding to the nearby boundary consisting of the uniform distribution of A or B units. An extra increment of energy must, therefore, be added to account for these non-uniformities which again is of the general form given by Eq. (14) in the vicinity of each relatively low Σ misorientation. When this energy is superimposed to obtain the final total energy (solid curve in Fig. 14) the result is a set of added cusps at the misorientations of the unfavored boundaries of relatively low Σ , i.e., at the points L, M and N, for example.

The energy changes which accompany the secondary relaxation may now be analyzed in the light of the above results. These energy changes in favored boundaries are zero in the present model, and, in principle, the favored boundaries may, therefore, be identified when $[E_R + E_P]$ is known as a function of θ as is the case, for example, in Fig. 8. The procedure is as follows. First, carry out the construction illustrated in Fig. 14 between every possible pair of boundary energy points in Fig. 8, on the assumption that each pair is a pair of favored boundaries and therefore of constant energies. The equilibrium boundaries will then be those boundaries corresponding to the lowest envelope of all of these curves.*

It is interesting to note that the $\Sigma=1$ boundary (i.e., the perfect lattice) will always be a favored boundary due to its low energy and that low angle boundaries near $\theta=0$, which are all high Σ boundaries, will be unfavored boundaries. The secondary relaxation which occurs in such low angle boundaries causes the units present in the low angle boundaries of high Σ to relax into structures which consist of mixtures of perfect lattice units and units of the next favored boundary which is present at larger θ .

* It is important to note that Sutton [27] has recently shown that it may be necessary to follow certain rules in selecting pairs of possible favored boundaries. This is due to the basic requirement that each pair of favored boundaries must be capable of producing all intermediate unfavored boundaries by the mixing of appropriate favored boundary units. Under certain conditions this requirement places a geometrical constraint on the choices of possible pairs of favored boundaries. For example, in the case of symmetric (001) tilt boundaries Sutton [27] has pointed out that two general types of boundaries exist, i.e., "centered" boundaries and "non-centered" boundaries. This leads to a requirement that at least one of every two adjacent favored boundaries must be centered. A detailed discussion of this problem is beyond the scope of the present paper and may be found in [27]. The main point to be made in the present context is that constraints of this type may exist on the choices of possible pairs of favored boundaries in the procedure described above.

7. CONCLUDING DISCUSSION

The present model has led to an $E(\theta)$ curve for [001] twist and tilt boundaries which consists of the very large cusp at small angles due to the primary relaxation and a series of smaller cusps at the larger angles at relatively low Σ misorientations due to the secondary relaxation. The average curve, therefore, increases from zero at $\theta=0$ and tends to level off at the larger angles if the perturbations due to the various smaller cusps are ignored. This type of curve has been found experimentally for [001] twist and tilt boundaries in copper by Gjostein and Rhines [28]. However, the cusps at the higher angles were not resolved in their work, and this may have been due to the existence of relatively weak cusps in copper and insufficient resolution in the experimental method to detect them clearly. We note in this respect that the decreases of energy at the low Σ misorientations in copper boundaries in Fig. 3 are relatively small, and that this would lead to relatively shallow cusps.

More generally, the present model seems consistent with the experimental and computational work reviewed in the Introduction indicating the existence of cusps in the $E(\theta)$ curve and arrays of SGBDs in non-favored boundaries.

It is anticipated that the main features of the present model should hold for other types of grain boundaries and interfaces even though the analysis may be more complicated. In the present [001] grain boundaries the primary relaxation is, fortunately, relatively simple, since it involves only one type of simple rotation. In the case, for example, of [110] grain boundaries the primary relaxation is undoubtedly more complex. Bollmann [1] has shown that three different O-Lattices (i.e., primary relaxations) must be involved if nearest-neighbor atoms in Lattices 1 and 2 in the vicinity of

each O-Lattice element are to be related over the full angular range by a transformation. At low angles up to $\theta = 20.1^\circ$ the O-Lattice corresponds to a simple rotational transformation of the type that applies to the [001] boundaries. Between $\theta = 20.1^\circ$ and 54.7° the transformation is more complex, except in the special case of the $\Sigma=9$ ($\theta=38.9^\circ$) misorientation where the transformation is a simple shear, and the O-Lattice becomes an array of parallel planes of zero shear. Between $\theta = 54.7^\circ$ and 90.0° the transformation again is more complex, except in the special case of the $\Sigma=3$ ($\theta = 70.5^\circ$) misorientation where the transformation again becomes a simple shear and the O-Lattice an array of parallel planes of zero shear. Ingle and Crocker [29] have calculated the relaxations which occur in the $\Sigma=3$ and $\Sigma=9$ [110] twist boundaries of copper. Their results for the $\Sigma=3$ boundary are illustrated in Fig. 15. They found that Lattice 2 translated off the CSL position, and as a result the transformation, A, relating nearest-neighbor atoms of Lattices 1 and 2, is a more complicated transformation consisting of a simple shear combined with a rigid body translation. The nearest-neighbor pairs related by this transformation are indicated in Fig. 15(a), along with the O-elements (planes of zero shear) and a Wigner-Seitz cell boundary between the O-elements. In the primary relaxation we therefore expect the paired atoms to move towards each other in the directions of the arrows in Fig. 15(a), and this is indeed closely the case as seen in Fig. 15(b) where the calculated results are shown. We note the interesting result that this pattern of primary relaxation is somewhat unexpectedly obeyed even in the region of the Wigner-Seitz cell boundary. Results for the $\Sigma=9$ boundary have also been published (see Fig. 3(b) of [29]), but in this case we have not been able to detect a clear indication of a primary relaxation corresponding to the expected transformation.

However, this may have been due to the fact that the $\Sigma=9$ boundary is not a favored boundary and that a relatively large secondary relaxation is present in the total relaxation which obscures the primary relaxation. In this respect it seems likely that the $\Sigma=3$ boundary in Fig. 15 is a favored boundary, and, hence, the primary relaxation is clearly revealed.

In the case of asymmetric tilt boundaries it has been shown [30] that the boundaries facet into units which are characteristic of symmetric tilt boundaries possessing the same crystal misorientation. This leads to the possibility of generalizing the present model to such boundaries. In addition, the geometry of interphase boundaries can be analyzed within the framework of the CSL model [31], and it, therefore, seems likely that the main concepts of the present model can be applied to such boundaries.

Finally, we mention that it would be highly desirable to have more extensive calculations over a wide range of boundaries to test further aspects of our proposed model.

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APPENDIX

METHOD FOR FINDING THE VECTORS BETWEEN THE ATOMS OF LATTICES 1 AND 2 ACROSS THE GRAIN BOUNDARY

A method for representing Lattice 1 or 2 in the frame of the DSC-Lattice has been developed recently [32]. The method used is to start with a Linear CSL cell of the type shown, for example, in Fig. A-1 for the case of $\Sigma=13$. The Linear CSL is defined for an (r,s) boundary plane (we work here in two dimensions) as a unit possessing Σ lattice points along the r,s direction in the DSC-Lattice frame. If we now superimpose the Lattice 2 points on this frame, it is easy to show that this Linear CSL cell is a repeating linear unit between two coincidence sites.

Each lattice point in this frame has the coordinates (mr,ms) where m takes integer values between 0 and $\Sigma-1$. As is shown in Fig. A-1, this Linear CSL passes through several conventional square CSL cells and is divided in that way into several segments. Each of these segments can be "folded" into the conventional square CSL cell at the origin by a translation corresponding to the CSL vector between the origin and the CSL cell in which it appears. This folding operation in the DSC-Lattice frame involves a translation consisting of integral numbers of Σ units in each direction of the base vectors of the CSL.

An alternative Linear CSL is the one which passes through $(\alpha_1, 1)$, shown in Fig. A-1. This follows from the result that there is always exactly one lattice point in each row/column of the DSC-Lattice frame within each conventional square CSL cell.

Having these results, we can represent the Lattice 1 points within one conventional square CSL cell as:

$$\vec{r}_1 = \begin{bmatrix} n_1 \alpha_1 \pmod{\Sigma} \\ n_1 \end{bmatrix} \quad \begin{matrix} \Sigma-1 \\ n_1 = 0 \end{matrix} \quad (A.1)$$

Here, the two components of $\vec{r}_1$ are along the edges of the CSL cell and are expressed in units of the DSC-Lattice. The quantity α_1 is the first component of $\vec{r}_1$, while the second component is equal to unity. In the same way, all vectors of Lattice 2 can be described as

$$\vec{r}_2 = \begin{pmatrix} -n_1\alpha_1 \pmod{\Sigma} + \Sigma\ell_1 \\ n_2 + \Sigma\ell_2 \end{pmatrix} \quad \begin{matrix} \Sigma-1 ; \infty \\ n_2 = 0 ; \ell_1, \ell_2 = -\infty \end{matrix}, \quad (\text{A.2})$$

and all the differences as

$$\vec{r}_1 - \vec{r}_2 = \begin{pmatrix} (n_1 + n_2)\alpha_1 \pmod{\Sigma} - \Sigma\ell_1 \\ (n_1 - n_2) \pmod{\Sigma} - \Sigma\ell_2 \end{pmatrix}. \quad (\text{A.3})$$

We have taken $(n_1 - n_2) \pmod{\Sigma}$ instead of $n_1 - n_2$ because ℓ_2 has the infinite indicated range in Eq. (A.2). Because $(n_1 - n_2) \pmod{\Sigma}$ covers all the numbers from 0 to $\Sigma-1$, and the sequence of the second component in Eq. (A.3) covers all integer values, we have to prove that for a given $(n_1 - n_2) \pmod{\Sigma}$ the first component exactly covers all integers. The proof is as follows:

$$n_1 + n_2 = n_1 - n_2 + 2n_2 = \text{given constant} + 2n_2.$$

By definition, Σ and 2 are relatively prime, and $n_2\alpha_1 \pmod{\Sigma}$ exactly covers all the integers. Therefore,

$$(n_1 + n_2)\alpha_1 \pmod{\Sigma}$$

exactly covers all integers.

In the case of a tilt boundary, ℓ_2 has a half infinite range, and, therefore, we do not have exact coverage of the DSC-Lattice. However, $\vec{r}_1 - \vec{r}_2$ still follow a characteristic pattern for each Σ as shown by Eq. (A.3) with $0 \leq \ell_1 < \infty$.

FIGURE CAPTIONS

- Fig. 1 (a) [001] planes of Lattices 1 and 2 in FCC crystal positioned on the $\Sigma=5$ CSL ($\theta = 36.9^\circ$) in configuration appropriate for twist boundary analysis. DSC-Lattice also shown. (b) Lattice of vectors, $\vec{R}_{ij}$, connecting atoms of Lattice 1 in CSL unit cell in (a) with all atoms of Lattice 2.
- Fig. 2 Minimum energy of [001] twist boundaries after the rigid body joining step, E_R , as a function of Σ . Results calculated for FCC and BCC structures using a Lennard-Jones and Johnson [13] potential respectively.
- Fig. 3 Minimum energy of [001] twist boundaries after the rigid body joining step, E_R , as a function of Σ . Results calculated for copper and nickel in [14].
- Fig. 4 Geometry of the integration method used for calculating the rigid body joining energy between the p^{th} plane of Lattice 1 and the l^{th} plane of Lattice 2 in a [001] twist boundary of large Σ .
- Fig. 5 Minimum energy of [001] symmetric tilt boundaries after the rigid body joining step, E_R , as a function of Σ . Results calculated for FCC and BCC structures using a Lennard-Jones and Johnson pairwise potential respectively. Indices of boundary plane indicated at top in each case.
- Fig. 6 Plot of minimum boundary energy after rigid body joining step, E_R , as a function of θ for the [001] twist boundaries in FCC structure with Lennard-Jones potential presented previously in

Fig. 2. Infinite number of points for high Σ boundaries shown as a row of closely spaced points.

Fig. 7 Schematic plot of primary relaxation energy, $E_p(\theta)$, as a function of θ for [001] twist boundaries corresponding to function given by Eq. (10). θ_c taken equal to $\pi/9$.

Fig. 8 Schematic plot of sum of rigid body joining and primary relaxation energies, $[E_R + E_p]$, as a function of θ for the [001] twist boundaries with the Lennard-Jones potential presented previously in Fig. 6. Infinite number of points for high Σ boundaries shown as line of closely spaced points.

Fig. 9 Schematic plot (cusped solid curves) of the total energies, $E = E_R + E_p + E_S$, near low Σ misorientations of the [001] twist boundaries presented previously in Fig. 8. Also shown are the energies $[E_R + E_p]$ of the high Σ boundaries transferred from Fig. 8 and the change in energy, E_S , associated with the secondary relaxation.

Fig. 10 Atomic displacements projected on boundary plane (vector arrows) associated with the total relaxation of [001] twist boundaries calculated by molecular statics [14]. Atoms in first planes of Lattices 1 and 2 above and below the boundary midplane are shown. Each displacement vector magnified 5 $\times$. (a) $\Sigma=5$ ($\theta=36.9^\circ$) boundary in copper. (b) $\Sigma=13$ ($\theta=22.6^\circ$) boundary in nickel. (c) $\Sigma=17$ ($\theta=28.1^\circ$) boundary in nickel. (d) $\Sigma=29$ ($\theta=16.3^\circ$) boundary in copper.

- Fig. 11 Atomic displacements associated with the total relaxation of $[001]$ $\Sigma=5$ ($\theta=36.9^\circ$) twist boundary in tungsten calculated by molecular statics in [20]. Atoms in first two planes of Lattices 1 and 2 above and below the boundary midplane are shown. O-elements are encircled. Arrows indicate rotational relaxations of Lattices 1 and 2 around the O-elements.
- Fig. 12 Atomic displacements in plane perpendicular to tilt axes (vector arrows) associated with the total relaxation of $[001]$ $\Sigma=5$ ($\theta=36.9^\circ$) tilt boundary in BCC iron calculated in present work by molecular statics using Johnson potential. Displacements magnified 400 $\times$.
- Fig. 13 Atomic displacements (vector arrows) resulting from insertion of a vacancy at atomic site indicated by circle in the $[001]$ $\Sigma=5$ twist boundary in tungsten shown previously in Fig. 11 (Results taken from [20].) Each cross centered on O-element.
- Fig. 14 Schematic plot of energies of unfavored boundaries between two favored boundaries at $\theta = \theta_A$ and $\theta = \theta_B$ respectively. Total energies at intermediate misorientations made up of self-energies of the favored boundary units and their interaction energy (dashed curve) plus the elastic energy in the adjoining lattices (see text). L, M and N are positions of unfavored boundaries of relatively low Σ . Numbers of A units and B units are equal at M.
- Fig. 15 Atomic displacements projected on boundary plane (vector arrows) associated with the relaxation of $[110]$ twist boundary ($\Sigma=3$, $\theta=70.5^\circ$) in copper. (a) Expected directions of displacements

associated with the primary relaxation. Lattice 2 is translated off the CSL position by translation calculated in [29] by molecular statics. Nearest-neighboring atoms of Lattices 1 and 2 connected by the transformation A are encircled. O-elements associated with transformation A are indicated.

(b) Actual total displacements ($2\times$) calculated by molecular statics in [29]. Only atoms in first planes of Lattices 1 and 2 above and below the boundary midplane are shown.

Fig. A-1 .Construction of conventional CSL from linear CSL for the $\Sigma=13$ ($r = 3, s = 2$) case (see text).

FIG. 1

FIG. 2

FIG. 3

FIG. 4

FIG. 5

FIG. 6

FIG. 7

FIG. 8

FIG. 9

FIG. 10(a)

FIG. 10(b)

FIG. 10(c)

FIG. 10(d)

FIG. 11

FIG. 12

FIG. 13

FIG. 14

FIG. 15

FIG. A-1