

Experimental evidence for a structural unit model of quasiperiodic grain boundaries in aluminum

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This paper presents a geometrical description of aperiodic grain boundaries within the framework of a quasiperiodic lattice. Experimental evidence is given in support of a structural unit model of quasiperiodic $[100]45^\circ$ twist and $[100]45^\circ$ twist plus tilt grain boundaries in aluminum.

I. INTRODUCTION

Grain boundary structures have been the subject of intensive theoretical and experimental investigations, ever since it was realized that they determine many physical properties in polycrystalline materials. The structure of grain boundaries has been described in terms of geometrical models based on the coincident site lattice (CSL),^{1,2} displacement shift complete lattice,²⁻⁴ and 0-lattice theories.³ Despite their usefulness in characterizing the global rigid nature of the grain boundary structure, these models still prove to be inadequate for providing a thorough representation of atomic relaxations that may occur at the grain boundary core. Moreover, these geometrical models are applicable only to periodic grain boundaries. Further advances in elucidating the relaxation processes have been achieved with the development of atomistic simulation methods. Methods such as molecular statics and molecular dynamics have been used extensively to model the structure of periodic grain boundaries.⁵

One significant aspect which emerges from the continued efforts to improve our knowledge of the structure of grain boundaries is the existence of some recurring structural units. The structural unit principle in grain boundaries was originally put forward by Bishop and Chalmers.⁶ Computer simulations of a large number of periodic grain boundaries in metals have placed the structural unit model on a sound foundation.⁷ Sutton and Vitek⁷ have also introduced rules for the determination of the sequence of structural units. This model, which involves structural units (SU), is equivalent to the secondary grain boundary dislocation (SGBD) concept, where a SGBD forms to accommodate the deviation from an "ordered interface".⁸

The Structural Unit/Grain Boundary Dislocation model (SU/GBD) for grain boundaries in cubic metals proposes the construction of any long period boundary from units of shorter period boundaries. These short period boundaries or "delimiting" boundaries fix the limits on the range of local misorientation. Long period boundaries in a range of misorientation may be

constructed with a mixture of these delimiting boundary units.

High-resolution electron microscopy (HREM) has provided experimental evidence for the structural unit model in periodic interfaces. Symmetrical $\langle 110 \rangle$ tilt boundaries,⁹⁻¹¹ $\langle 001 \rangle$ tilt boundaries,¹² and $\langle 111 \rangle$ tilt boundaries in gold¹³ have shown the existence of low energy basic structural units.

Despite these advances in the structural characterization of simple periodic interfaces, the structure of complex general grain boundaries remains a challenge. Quasiperiodic interfaces may provide a link between the simple periodic grain boundaries and the most general grain boundaries. The concept of quasiperiodicity at interfaces was first introduced by Rivier.¹⁴ Sutton has used the framework of the structural unit model to describe irrational tilt grain boundaries as one-dimensional quasicrystals.¹⁵ He has also shown that the "strip and projection" method for generating quasiperiodic lattices¹⁶ produces sequences of structural units identical to the algorithm introduced by Sutton and Vitek in Ref. 7. Independently, Gratias and Thalal¹⁷ have shown that all grain boundaries (coincidence lattice or general) can be constructed by projecting a periodic six-dimensional lattice in a three-dimensional space. This three-dimensional cut is the dichromatic pattern (DCP), and is dependent upon the relative misorientation of the grains. The six-dimensional lattice, however, is independent of the actual boundary, with the misorientation characterized completely by the projection matrix. Sutton¹⁸ has generalized these concepts for heterophase interfaces. Rivier and Lawrence showed that a general grain boundary is composed of a quasilattice of topological dislocations.¹⁹

While the theoretical basis of quasiperiodic interfaces is now well established, there are limited experimental examples to support it. Recently, experimental evidence has been presented for the support of a structural unit model in an aperiodic grain boundary in aluminum.²⁰ The misorientation of the bicrystal was characterized by a $[100]45^\circ$ rotation followed by a 17.5°

rotation about a $\langle 001 \rangle$ and $\langle 011 \rangle$ direction common to the two abutting crystals. The structure of the grain boundary in the 17.5° rotated bicrystal was described in terms of a mixture of two basic structural units corresponding to the delimiting misorientations of 13.79° and 19.47° . In this paper we present experimental illustrations favoring the concept of structural units in quasiperiodic grain boundaries.

II. TWO-DIMENSIONAL QUASIPERIODICITY: THE CASE OF THE $45^\circ[100]$ MISORIENTATION

Figure 1 is a HREM image of a $45^\circ (\pm 1.5^\circ)$ $[100]$ misoriented aluminum bicrystal with a grain boundary approximately parallel to the $(11\bar{1})$ plane of crystal 1. The bicrystal was prepared by strain-annealing 99.999% pure aluminum single crystals.²¹ The high resolution electron micrograph was recorded with a JEM-4000EX operated at 400 kV near the optimum defocus at a magnification of 500 000. Under these experimental conditions, the atomic columns appear black.

Figure 2(a) represents the dichromatic pattern (DCP) for the $[100]45^\circ$ misorientation between two face-centered-cubic crystals as viewed along the $[100]$ rotation axis. A view of this same DCP along the common $[011]$ direction of crystal 1 (black atoms) and $[001]$ direction of crystal 2 (white atoms) is given in Fig. 2(b).

The DCP exhibits an $8'/m 2/m 2'/m'$ point group symmetry, where the operations of symmetry indicated with a prime are colored operations relating atoms of different color belonging to the two interpenetrated crystals.²² The unprimed operations of symmetry relate atoms within their respective lattice. The eightfold colored axis is parallel to the rotation axis with a mirror

plane parallel to the (100) plane. Three mirror planes perpendicular to twofold axes are coplanar with the $\{110\}$ and $\{100\}$ planes common to both lattices. The unit vector

$$\mathbf{u} = \left(1 - \frac{1}{\sqrt{2}}\right)^{-1/2} \begin{bmatrix} 0 \\ \sqrt{2} - 1 \\ 1 \end{bmatrix}$$

and its symmetry related counterparts (as referred to the lattice of crystal 1) are parallel and perpendicular to colored twofold axes and colored mirror planes.

The $45^\circ[100]$ DCP is periodic along the rotation axis. However, the octahedral symmetry of the two-dimensional projection of the DCP onto the (100) plane is inconsistent with periodicity within that plane. The coincident site lattice (CSL), displacement shift complete lattice (DSC), and 0-lattice therefore become unsuitable for the geometrical characterization of the $[100]45^\circ$ misorientation. The reciprocal of the density of coincident points, Σ , assumes an infinite value, while the DSC lattice vectors become infinitely small. Despite the lack of periodicity, the $[100]45^\circ$ DCP does possess some useful properties. If we define by $\mathbf{r}_1\{x_1, y_1\}$ a site in the (100) plane of lattice 1, the site $\mathbf{r}_2\{x_2, y_2\}$ in the (100) plane of lattice 2 transforms to

$$\mathbf{r}'_2 \left\{ x'_1 = \frac{1}{\sqrt{2}}(x_2 + y_2), y'_1 = \frac{1}{\sqrt{2}}(-x_2 + y_2) \right\}$$

after a 45° rotation with respect to lattice 1.

Aside from the origin, the distance between any two such lattice points of the DCP is strictly greater than zero (i.e., there is no other coincident point). However, for any given $\epsilon > 0$, there exist a set of lattice translations, \mathbf{T} , within the (100) plane of lattice 1 such that $|\mathbf{r}'_2 - \mathbf{T}| < \epsilon$; that is, one can always find two

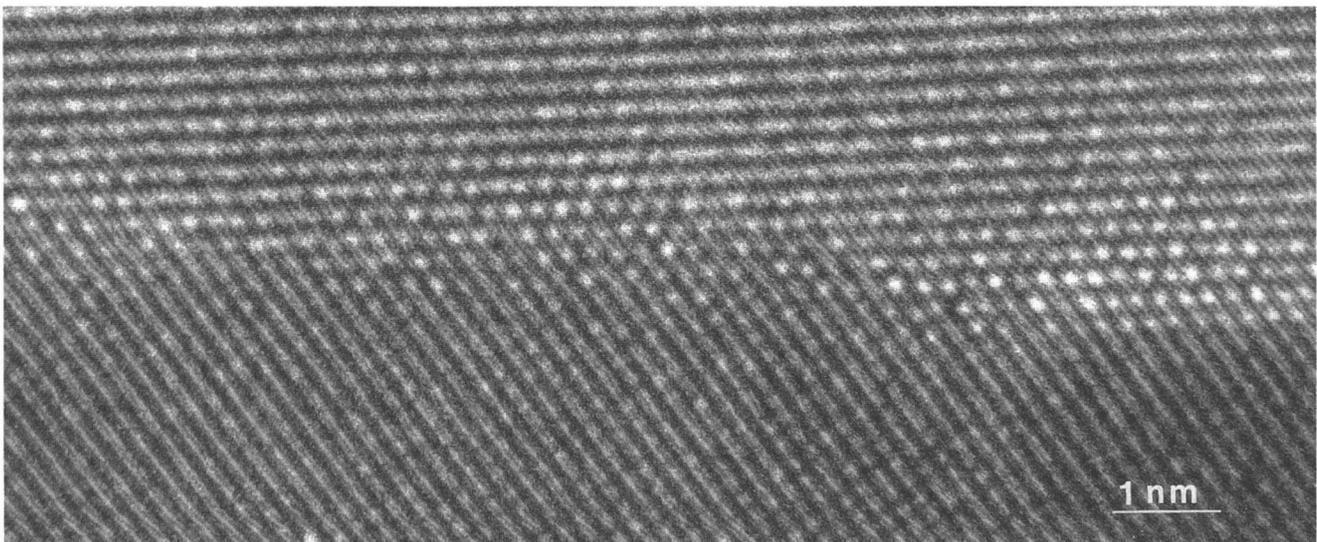


FIG. 1. HREM micrograph of a $45^\circ[100]$ bicrystal as viewed along the directions $\langle 100 \rangle_1 \langle 110 \rangle_2$ common to both grains.

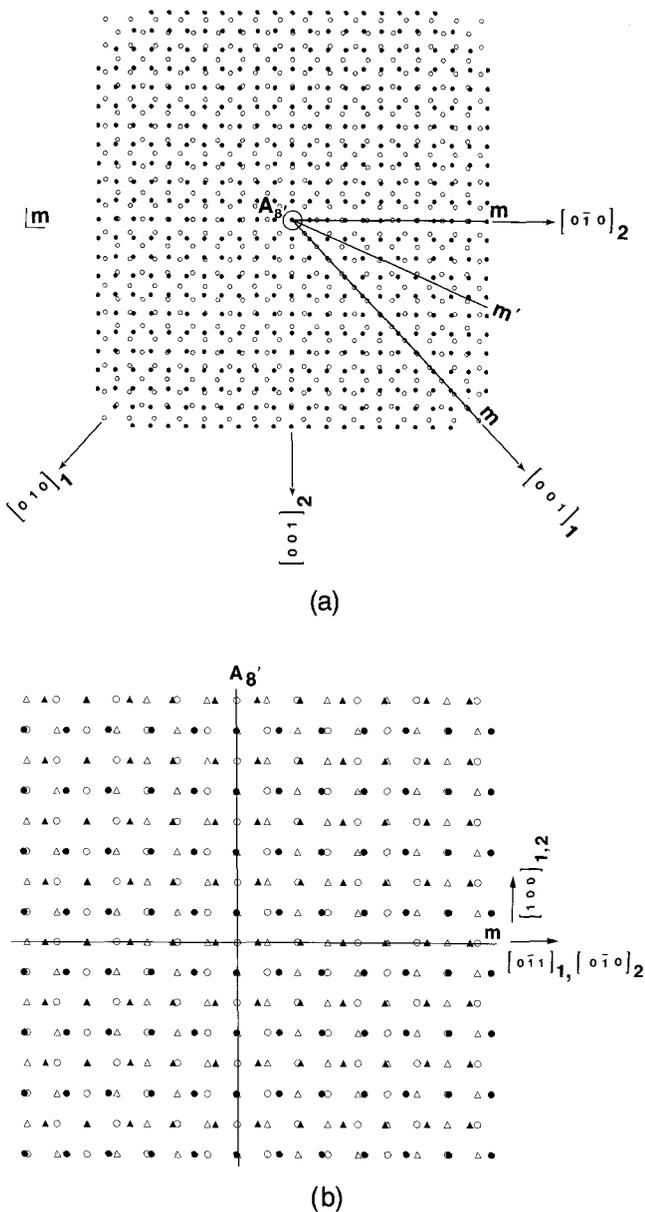


FIG. 2. (a) 45°[100] dichromatic pattern as viewed along the [100] direction. The filled and unfilled circles correspond to lattices 1 and 2, respectively. (b) 45°[100] dichromatic pattern viewed along $[001]_2$ or $[011]_1$. The filled and unfilled circles and triangles represent successive $(001)_2$ and $(011)_1$ planes.

sites in the two interpenetrated crystals such that their distance is less than some positive number arbitrarily small. For example, if one considers the one-dimensional case along the $[001]$ direction of lattice 1, the lattice sites $r_2\{x_2, y_2\}$: $(1.5, 1.5)$; $(3.5, 3.5)$; $(5, 5)$; $(7, 7)$; $(8.5, 8.5) \dots$ are all within $\epsilon = 0.15$ of lattice 1 sites: $(0, 2)$; $(0, 5)$; $(0, 7)$; $(0, 9)$; $(0, 12) \dots$. The 45°[100] DCP is not periodic as ϵ is always a nonzero number, but rather it possesses a quasiperiodic nature.²³ This quasiperiodic DCP is compatible with the octahedral symmetry.

A two-dimensional quasiperiodic lattice with symmetry $8m$ can be constructed by projection of a four-dimensional hypercubic lattice onto a two-dimensional plane with indices that are in the ratio of the irrational number $\sqrt{2} + 1$.²⁴ The two-dimensional plane is filled by a set of two unit cells: a square and a rhombus with matching edges (see Fig. 3). This construction is similar to the Penrose quasiperiodic tiling of a plane with fivefold symmetry.²⁵

Following Gratias and Thalal,¹⁷ the two-dimensional 45°[100] DCP of Fig. 2(a) can also be recovered by projecting a four-dimensional lattice [with natural basis $E_1 = (1, 0, 0, 0)$, $E_2 = (0, 1, 0, 0)$, $E_3 = (0, 0, 1, 0)$, and $E_4 = (0, 0, 0, 1)$] onto a two-dimensional plane by using the 4×2 projection matrix:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Theoretically the (100) plane can be filled in by tiles of any size. Since we wish to use the quasiperiodic tiling as a reference frame for the DCP, we need to impose a relationship between the octahedral quasiperiodic tiling and the 45°[100] DCP. To achieve that goal, we superpose the squares and rhombuses onto the DCP such that all edges of the tiles are parallel to the colored mirror planes. We also impose a constraint on the size of the tiles, requiring that every tile possess two opposite vertices lying between two differently colored lattice sites. Thus, in Fig. 4, the minimum length of the edges of the tiling unit cells is

$$L = \frac{a}{4\sqrt{2} \cos \frac{45^\circ}{4}} (\sqrt{2} + 1)$$

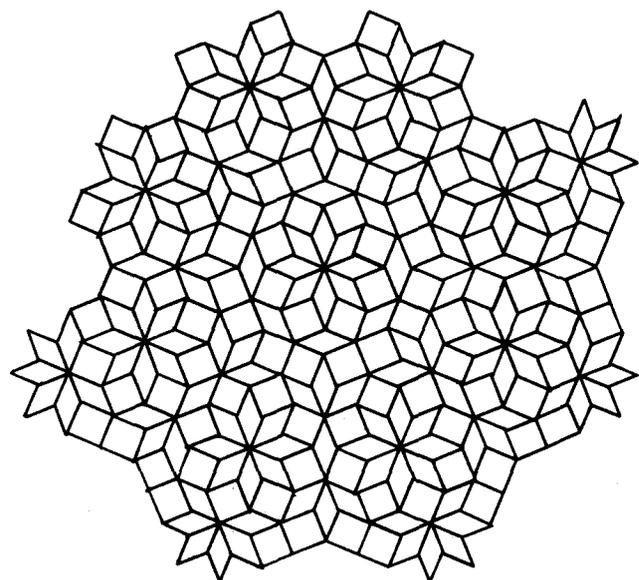


FIG. 3. Octahedral quasiperiodic tiling of the plane with square and rhombus unit cells.

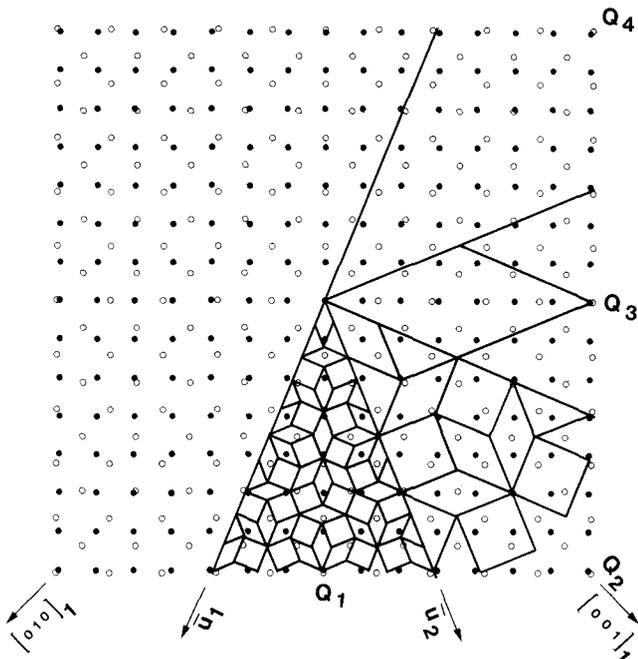


FIG. 4. Superposition of quasiperiodic tiling onto $45^\circ[100]$ dichromatic pattern. The octants Q_1, Q_2, Q_3, Q_4 correspond to successive application of the inflation rule of quasiperiodic lattices.

where a is the lattice parameter.

This constraint leads to a direct relationship between the atomic structure of the DCP and the quasiperiodic tiling. The lattice positions of the two-dimensional quasiperiodic tiling are given by a set of vectors, \mathbf{x}_i , such that $\mathbf{x} \cdot \mathbf{u}_i = x_{im}$.²³ Here m runs over all integers and \mathbf{u}_i are unit vectors along the axes of a regular octahedron. Two of these unit vectors delimiting the lower half octant of the plane are:

$$\mathbf{u}_1 = \left(1 - \frac{1}{\sqrt{2}}\right)^{-1/2} [\sqrt{2} - 1, 1]$$

and

$$\mathbf{u}_2 = \left(1 - \frac{1}{\sqrt{2}}\right)^{-1/2} [(1, \sqrt{2} - 1)]$$

referenced to crystal 1 (see Fig. 4). The coordinates of the quasiperiodic lattice points (vertices) along each axis of the octahedron are defined by a quasiperiodic sequence of two incommensurate intervals, L_1 and L_2 , in the ratio $L_1/L_2 = \sqrt{2} + 1$. The number of intervals or equivalently the number of squares to rhombuses is in the same ratio. This ratio is the solution of the second order polynomial equation $x^2 - 2x - 1 = 0$.

The sequence of intervals along each axis is also characterized by a substitution law $L'_i = M_{ij}L_j$ where $i, j = 1, 2$ and the substitution matrix is

$$[M_{ij}] = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}.$$

The substitution of an interval L'_1 for a segment $2L_1 + L_2$ and an interval L'_2 for a segment L_1 , allows the creation of another quasiperiodic lattice constituted of larger unit cells. These cells have the same ratio as before, $L'_1/L'_2 = \sqrt{2} + 1$. With this substitution, all previous properties of the quasiperiodic lattice, including symmetry, are conserved.

Because of the imposed relationship between the quasiperiodic lattice and the DCP, opposite vertices of inflated unit cells again mark midpoints between oppositely colored atomic sites. The pairs of colored atomic sites located at tile vertices of the quasiperiodic lattice show a higher degree of "coincidence" upon subsequent inflation. This property may be illustrated by the variation of the degree of coincidence along the $[001]$ direction of crystal lattice 1. The distance between the colored atoms located about the vertex of the first rhombus (from the origin in Fig. 4) measures 17% of one atomic spacing. Upon successive inflation, the vertex of the first rhombus falls between pairs of colored atoms separated by 7%, 2.94%, ... of one atomic spacing.

Repeating the inflation rule to infinity leads to almost perfect coincidence between atoms at an infinite distance from the origin. The quasiperiodic octahedral lattice provides a measure of the degree of lattice match, as well as a map of locations within the DCP with any given degree of coincidence.

Parallel to the inflation rule is the approximation of the irrational number $\sqrt{2} + 1$ by a sequence of rational numbers. These rational numbers correspond to successive periodic approximations of the exact quasiperiodic $45^\circ[100]$ misorientation.

All CSL formed by rotation, α , about $[100]$ can be obtained from the generating functions:

$$\Sigma = r^2 + s^2 \quad \text{when } r^2 + s^2 \text{ is an odd number}$$

$$\Sigma = \frac{r^2 + s^2}{2} \quad \text{when } r^2 + s^2 \text{ is an even number}$$

and

$$\alpha = 2 \tan^{-1} \left(\frac{s}{r} \right).$$

The sequence $r/s = 2/1, 5/2, 12/5, 29/12, \dots$ approximates $\sqrt{2} + 1$. This corresponds equivalently to the series $\Sigma = 5(\alpha = 36.869^\circ), \Sigma = 29(\alpha = 43.600^\circ), \Sigma = 169(\alpha = 44.780^\circ), \Sigma = 985(\alpha = 44.959^\circ), \dots$ approximating the $\Sigma = \infty(\alpha = 45^\circ)$ misorientation. This sequence $\Sigma = 5, 29, 169, 985, \dots$, constitutes a series of delimiting misorientations of ever decreasing range centered on the 45° rotation angle.

The concept of sequential rational approximations to the irrational misorientation is elucidated by examining the plane spacings in the HREM image of Fig. 5. As anticipated, the bicrystal exhibits continuity of the $(010)_2$ and $(011)_1$ crystal planes. In the vicinity of

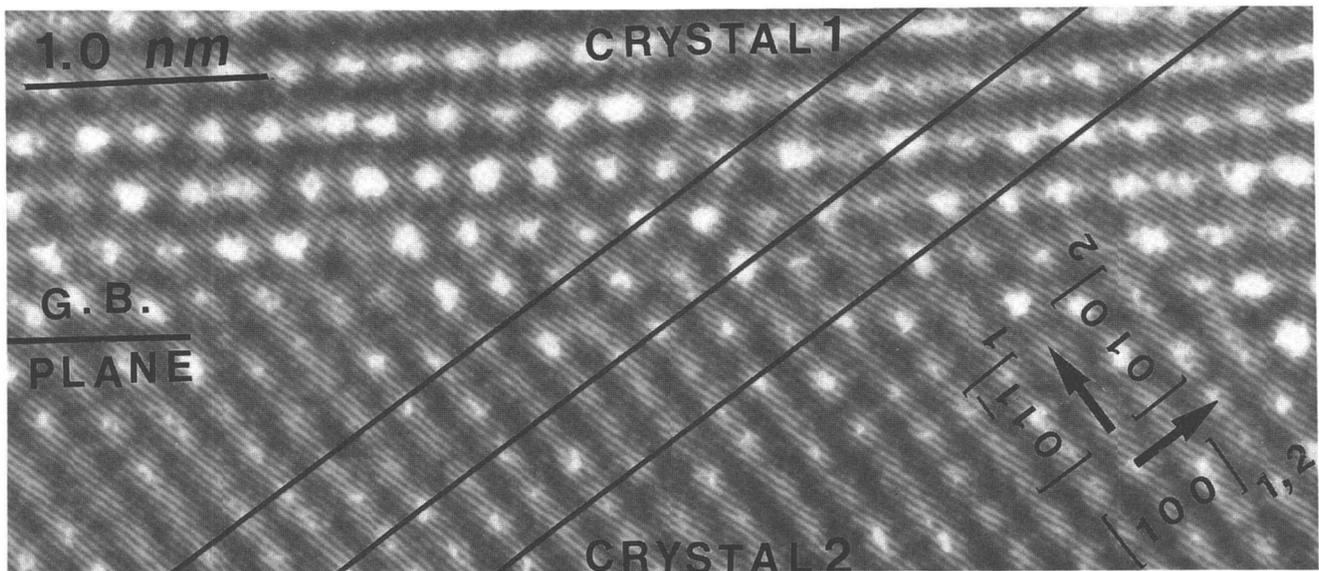


FIG. 5. HREM micrograph of a segment of a $45^\circ[100]$ bicrystal. The grain boundary segment is parallel to the $(11\bar{1})$ plane. The lines show continuity of the $(010)_2$ and $(01\bar{1})_1$ planes across the interface.

the grain boundary core, the $(010)_2$ and $(01\bar{1})_1$ planes match every 2 and 3 respective interplanar spacings. The rational number $3/2$ is an approximation to the irrational interplanar spacing ratio of $\sqrt{2}$. In the CSL description, $3/2$ is equivalent to the ratio $5/2$ in the r/s sequence. In other words, the observed match between the $(010)_2$ and $(01\bar{1})_1$ planes is representative of a $\Sigma = 29$ ($\alpha = 43\ 600^\circ$) structural unit composition of the irrational interface. One cannot construct the $45^\circ[100]$ grain boundary with $\Sigma = 29$ units alone, however, since $3/2$ is only an approximation to $\sqrt{2}$. We hypothesize that the grain boundary should also contain other short length structural units. A good candidate for this is the $\Sigma = 5$ unit,⁸ corresponding to the CSL ratio $r/s = 2/1$. While we are still investigating, we have not yet identified such a unit in the HREM image of the 45° twist grain boundary (Fig. 5).

III. THREE-DIMENSIONAL QUASIPERIODIC DCP

We now consider the effect of a rotation, θ , about the $[011]_1 \parallel [001]_2$ axes. Figure 6 shows a high resolution electron micrograph of a $[100]45^\circ$ twist plus $\theta \cong 17.5^\circ$ tilt grain boundary in aluminum. The asymmetric grain boundary is parallel to the $(010)_2$ or $(499)_1$ planes. The introduction of the additional rotation results in a decrease of the DCP group symmetry from $8'/m\ 2'/m'\ 2/m$ to $2'/m'\ 2'/m'\ 2/m$. This supplemental rotation also destroys the periodicity of the DCP along the $[100]$ axis. By inspection, one can find special rotations that may be referred to as quasiperiodic lattices with small dimension unit cells (or tiles). We use as an

example, $\theta = 13.29^\circ$, which aligns the (010) plane of crystal 2 with the $(1\bar{3}3)$ plane of crystal 1.

For the sake of simplicity, we construct a one-dimensional DCP from the three-dimensional one. We first superpose the $(1\bar{3}3)_1$ and $(010)_2$ planes onto a single plane, producing a two-dimensional DCP. The atomic content of the two-dimensional DCP is then projected onto the line $[3\bar{1}1]_1$ (or $[100]_2$). This one-dimensional DCP is characteristic of the atomic matching along the grain boundary plane. We call d_1 the spacing between black atoms (of lattice 1) in the one-dimensional DCP. Similarly, d_2 corresponds to the white atom spacings. The ratio, d_1/d_2 , is then given by the irrational value of $\sqrt{19/2}$. The quasiperiodic one-dimensional DCP is characterized within a one-dimensional quasiperiodic lattice constituted of two incommensurate intervals. The lengths of the two intervals, L_1 and L_2 , are in the irrational ratio of $\sqrt{19/2} + 3$. All lattice points in this one-dimensional quasiperiodic lattice fall midway between two differently colored atomic sites.

The ratio L_1/L_2 satisfies the second order polynomial equation $2x^2 - 12x - 1 = 0$. This equation yields the recurring scheme for successive approximants, a_n and a_{n+1} , of L_1/L_2 :

$$a_{n+1} = \frac{1}{2a_n} + 6$$

The sequence of rational numbers $6/1, 73/2, 444/73, \dots$, approximates the irrational number $\sqrt{19/2} + 3$. The ratio, d_1/d_2 , is approximated by $3/1, 37/12, 275/73, \dots$, corresponding to increasingly better degrees of

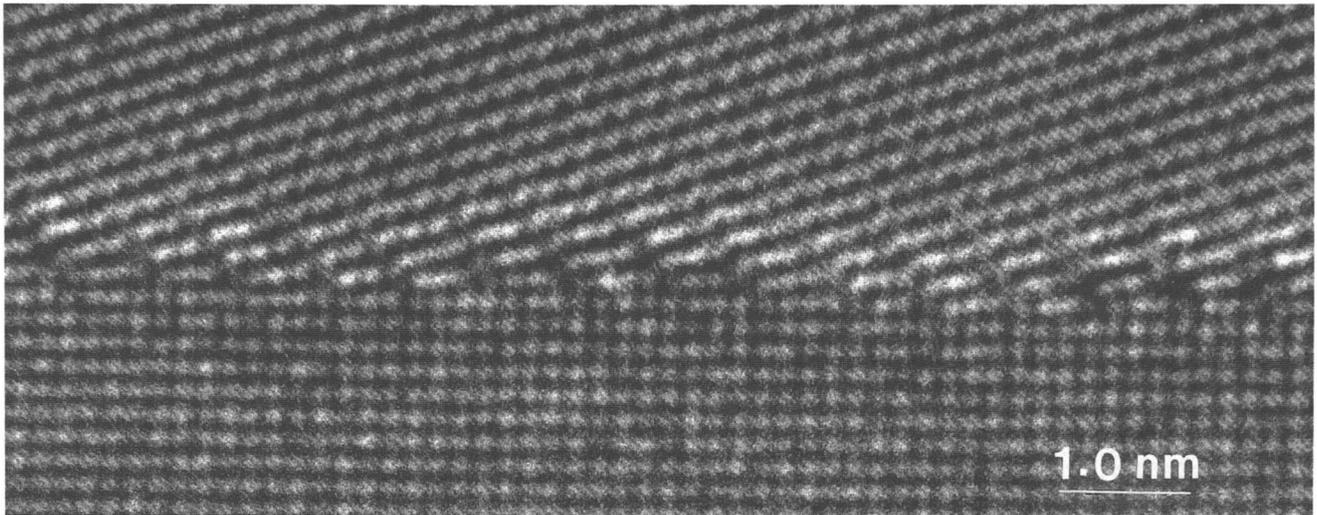


FIG. 6. HREM micrograph of $45^\circ[100]$ plus $\theta \simeq 17.5^\circ [001]_2 \parallel [011]_1$.

coincidence along the one-dimensional DCP. In Table I, we list a few of the rotations, θ , and their corresponding d_1/d_2 first approximants.

The quasiperiodic lattice characteristics for a $\theta = 17.44^\circ$ misorientation are $d_1/d_2 = 2\sqrt{89}$, $L_1/L_2 = 2(\sqrt{89} + 9)$, with a second order polynomial equation $x^2 - 36x - 32 = 0$. The ratio of d_1/d_2 is approximated by the sequence of rational numbers: $18/1, 170/9, \dots$

A first approximation to the atomic spacing ratio of $18/1$ demonstrates the long quasiperiodic nature of the DCP along the $[9\bar{4}4]_1$ and $[010]_2$ directions. Figure 7 represents a possible atomic arrangement in the grain boundary core drawn from the micrograph of Fig. 6. The grain boundary appears to be composed of a mixture of two types of short structural units, corresponding to the $\theta = 13.29^\circ$ ($3/1$) and $\theta = 19.47^\circ$ ($4/1$) first approximations. The proximity of $\theta = 17.44^\circ$ to the 19.47° rotation imposes a greater frequency of ($4/1$) structural units than ($3/1$) units. The algorithm of Sutton¹⁵ or Sutton and Vitek⁷ may be used to determine the sequence of structural units in the quasiperiodic interface. We label *A* and *B* the delimiting units ($3/1$) and ($4/1$), respectively. The sequence of these units using the rational approximant, $18/1$, for the irrational ratio, d_1/d_2 , may be obtained by using 2 *A* units and 3 *B* units.

Since $1/2 < 2/3 < 1/1$, the boundary is con-

stituted of longer units $C = ABB$ and $D = AB$, in the ratio $1/1$. The corresponding boundary is then described periodically by repeating the sequence $\dots ABBAB \dots$. We can generate a better approximation for the quasiperiodic grain boundary by considering the sequence of 36 *A* units and 143 *B* units, corresponding to the next rational approximant, $d_1/d_2 = 170/9$. Since $1/4 < 36/143 < 1/3$, boundary is composed of a sequence of $C = ABBBB$ and $D = AB BB$ units. The *C* and *D* units are in a ratio of 35 to 1. The complete quasiperiodic sequence of units may be produced at the limit of the rational series. At that point, however, the number of units then becomes impractical for use. The segment of grain boundary resolvable in the high resolution electron micrograph is too limited in size to allow us to make a definitive conclusion about the irrational sequence of structural units.

Finally, we note that a $\theta = 35.26^\circ$ (the quasiperiodic characteristics are given in Table I) may be constructed with two short length structural units, namely $2/1$ and $5/2$ units. Contrary to the case of $\theta = 17.44^\circ$, these two units are not delimiting units.

IV. CONCLUSION

In this paper, we have discussed an application of the structural unit model of grain boundaries to quasiperiodic interfaces. A quasiperiodic tiling representation

TABLE I. Quasiperiodic properties of some $45^\circ[110]$, $\theta[001]_2 \parallel [011]_1$ misorientations.

GB plane	θ	d_1/d_2	L_1/L_2	2nd order polynomial	L_1 rational sequence d_1/d_2
($\bar{1}\bar{3}\bar{3}$)	13.29°	$\sqrt{19/2}$	$\sqrt{19/2} + 3$	$2x^2 - 12x - 1 = 0$	$3/1, 37/12, 225/73, \dots$
($\bar{1}\bar{2}\bar{2}$)	19.47°	$3\sqrt{2}$	$3\sqrt{2} + 4$	$x^2 - 8x - 2 = 0$	$4/1, 17/4, 140/33, \dots$
($\bar{1}\bar{1}\bar{1}$)	35.26°	$\sqrt{6}$	$\sqrt{6} + 2$	$x^2 - 4x - 2 = 0$	$2/1, 5/2, 22/9, \dots$

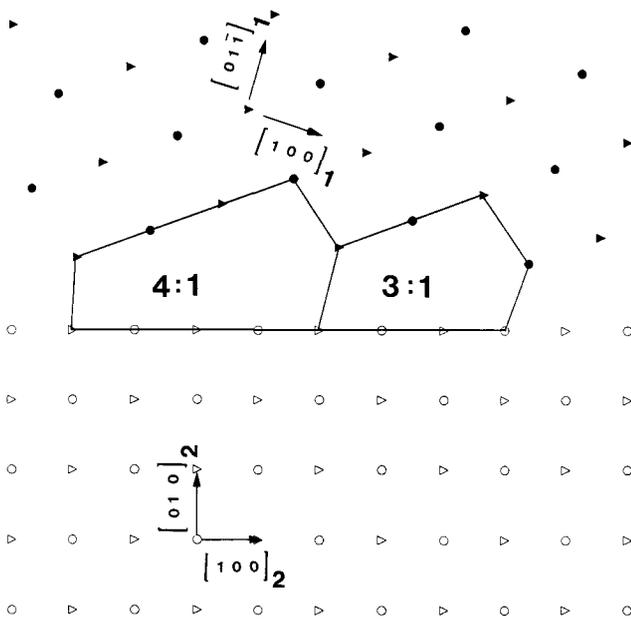


FIG. 7. Schematic representation of the grain boundary of Fig. 5. ●, ○, △, ▲ are atoms in successive planes.

for nonperiodic grain boundaries offers a suitable frame for the geometrical description of such boundaries. The size of the tiles is constrained by a simple relationship between the quasiperiodic lattice and quasiperiodic DCP. We have also provided experimental evidence for the relaxation of quasiperiodic grain boundaries into short period structural units. From our observation, it appears that long quasiperiodic boundaries may be constituted of a mixture of short length structural units. The short length units are representative structural units of short period or quasiperiodic delimiting grain boundaries.

The structural unit model of a grain boundary requires that there exist an infinite number of structurally similar regions susceptible to relaxation into the structural units. While periodicity is a sufficient condition to support a structural unit model, it is in no way obvious that quasiperiodic boundaries may be described in those terms. Central to this point is the property of local pattern density in quasiperiodic tiling. Sutton has recognized that the local pattern density (or local isomorphism) at quasiperiodic interfaces is similar to the property of translational invariance at periodic interfaces.¹⁸

The local isomorphism property of quasiperiodic lattices^{16,26} states that any finite patch of tiles that belongs to the quasiperiodic lattice appears infinitely many times. It is important to consider how far apart two identical patches are in a particular quasiperiodic lattice. If d is the diameter of a given patch, $2d$ represents an upper bound for the distance at which an identical patch may be found.²⁷ This holds true, however, only if the irrational number is an algebraic number. The exceptions are the Liouville numbers for which the

distance may grow arbitrarily quickly.¹⁶ The property of local pattern duplication makes the representation of the infinite period $45^\circ[100]$ twist plus tilt boundaries in terms of short period structural units a viable concept. Indeed, all the grain boundaries discussed in this paper correspond to algebraic quadratic irrational numbers.

From an energetic point of view, the inflation rule/degree of coincidence property of the quasiperiodic lattice and $45^\circ[100]$ DCP allows a quantitative measure of atomic displacement necessary for the relaxation to shorter period structural units. However, the description of a $45^\circ[100]$ twist quasiperiodic boundary in terms of any one of the short period boundaries will depend upon the details of interatomic forces.

Recently, the two structural units (3/1) and (4/1) for the $45^\circ[100]$ twist plus 13.29° and 19.47° tilt grain boundaries in aluminum have been studied by molecular dynamics.²⁸ The interatomic forces between aluminum atoms were modeled by the use of density dependent pseudopotentials. The structural units have proven to be stable and to undergo only limited relaxation. The computer models, therefore, support the existence of structural units in the 17.44° tilt grain boundary. Moreover, along the $[011]_1$ and $[001]_2$ directions, the simulated bicrystals clearly exhibit plane matching every 3 and 2 or 1 and 1, respective interplanar spacing. This observation is an illustration of a $\Sigma 5$ and $\Sigma 29$ structural unit composition for a quasiperiodic bicrystal with the characteristic irrational number $\sqrt{2}$.

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