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COINCIDENCE IN RECTANGULAR LATTICES.(U)

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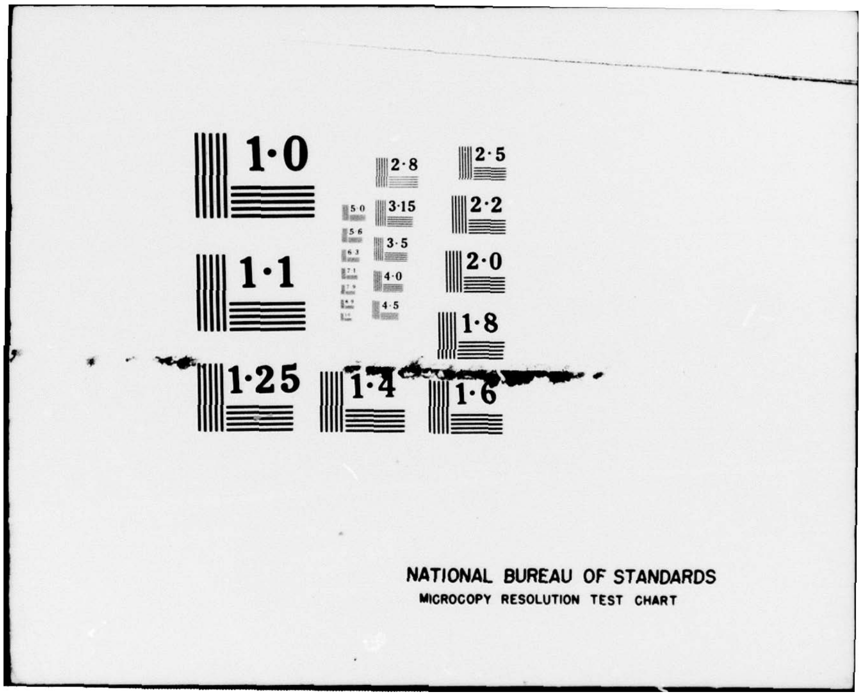
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COINCIDENCE IN RECTANGULAR LATTICES

GORDON A. BRUGGEMAN and GEORGE H. BISHOP, Jr.
MATERIALS SCIENCES DIVISION

February 1977

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ARMY MATERIALS AND MECHANICS RESEARCH CENTER
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ABSTRACT

The conditions for the formation of rows of coincidence sites in two-dimensional rectangular lattices (equivalent to forming two-dimensional arrays of coincidence sites in real crystals) are considered for varying values of the axial ratio. The crystallographic relations leading to such coincidence rows are far less restrictive than those required for the formation of coincidence-site lattices (CSL's). The complete-pattern-shift lattice (DSC lattice), which defines the pattern-preserving displacements of one crystal relative to the other for a given coincidence array, degenerates into a series of parallel lines from a series of discrete points as the coincidence array changes from a two-dimensional to a one-dimensional pattern in misoriented planar lattices, or from a CSL to a two-dimensional array in misoriented three-dimensional crystals. The apparent freedom of definition in the pattern-preserving displacements for these lower-order coincidence arrays is without physical significance to real grain boundary structures, however, in that conditions must not be too far removed from those of exact coincidence for meaningful pattern-preserving displacements to be obtained. Thus, although two-dimensional coincidence arrays are able to occur quite generally, even in crystals of lower symmetry, their significance to general boundary structures is limited unless they can be associated with a near-coincidence relationship.

INTRODUCTION

The concepts of near-coincidence and of near-coincidence-site lattices (near-CSL's) have previously been introduced to describe in noncubic crystals (principally hcp crystals) the analog to exact coincidence and exact coincidence-site lattices that occur in cubic crystals.[1] The three-dimensional arrays of exact coincidence sites characteristic of the latter cannot be produced in noncubic lattices except when certain crystallographic conditions are fulfilled (e.g., in hcp or tetragonal crystals, $(c/a)^2$ must be a rational number). However, it has been suggested that only two-dimensional arrays of coincidence sites have significance in grain boundaries, and that therefore the concept of near-coincidence is of questionable importance to general considerations of grain boundary structure.[2] It is true that the conditions for achieving two-dimensional arrays of coincidence sites are far less stringent than those for achieving three-dimensional coincidence, implying a distinction of particular importance to possible boundary structures in noncubic lattices. Nevertheless, it will be shown in this report that the ease of achieving two-dimensional coincidence arrays does not mitigate the need for three-dimensional near-coincidence in describing the structure of special boundaries in noncubic crystals.

Any twinning operation (i.e., a 180° rotation about the normal to the twin plane) will generate a two-dimensional coincidence array in the twin plane or likewise, in lattice of appropriate symmetry, rotations of one lattice plane into exact coincidences with the equivalent lattice plane reflected across a mirror plane of the lattice will lead to two-dimensional coincidence arrays. Such two-dimensional arrays have been termed two-dimensional CSL's.[2] It is the preservation of such periodic arrays in coincidence and off-coincidence grain boundary structures that presumably imparts lower grain boundary energy. Two-dimensional CSL's abound in crystals that exhibit exact three-dimensional coincidence; as many as 9 percent of the boundaries in a *random* polycrystalline aggregate would lie within the assumed energy cusps at coincidence misorientations in cubic crystals for example,[3] even more when coincidence is a factor in nucleation and growth selection. However, in crystals that fail to exhibit exact three-dimensional coincidence, exact two-dimensional arrays of coincidence sites have been shown to commonly occur only in symmetric and pseudo-symmetric tilt boundaries or in certain twist boundaries.* Nevertheless, the possibilities for the existence of coincidence grain boundaries in noncubic crystals are far more numerous than previously supposed.

In this report, the various levels of coincidence that can be achieved in two-dimensional rectangular lattice are treated. The formation of two-dimensional coincidence arrays in such a two-dimensional lattice is analogous to forming three-dimensional arrays (CSL's) in a three-dimensional crystal. Furthermore, the two-dimensional CSL's of three-dimensional crystals have their counterparts in one-dimensional "coincidence rows" in a two-dimensional lattice. Since many crystal structures can be built up from the uniform stacking of layers of atoms laid out

1. BRUGGEMAN, G. A., BISHOP, G. H., Jr., and HARTT, W. H. *Coincidence and Near-Coincidence Grain Boundaries in HCP Metals*, in the Nature and Behavior of Grain Boundaries, ed., H. Hu, Plenum, 1972, p. 83-122.
2. LOBERG, B., and SMITH, D. A. *Periodic Structures and Grain Boundaries in Magnesium*. J. Microscopy, v. 102, 1974, p. 317-322.
3. WARRINGTON, D. H. *Special Grain Boundaries in Random Polycrystalline Aggregates*. J. Microscopy, v. 102, 1974, p. 301-308.

*Pseudo-symmetric boundaries are tilt boundaries in which sites on the Bravais lattices of each crystal are mirror images of one another, but in which only some but not all *atomic sites* are symmetrically disposed (Reference 1).

on rectangular networks, the misorientation relationships which produce coincidence in the two-dimensional rectangular lattice will coincide with the misorientation relationships which produce coincidence in the three-dimensional crystal for rotations about the normal to the particular crystallographic plane. Two-dimensional coincidence arrays in the plane of the rectangular lattice automatically correspond with a CSL in the three-dimensional crystal when there is a repetitive sequence in the stacked layers. This is invariably the case, for example, in cubic crystals, in hcp and tetragonal crystals with rational values of $(c/a)^2$, and when the stacked layers correspond to crystallographic planes normal to or in the zone of the c-axis when $(c/a)^2$ is irrational. Similarly, "coincidence rows" in two dimensions correspond with two-dimensional CSL's in three dimensions under the same circumstances. When the stacked layers do not repeat, however, any coincidence that occurs will generally be confined to a single layer. This report considers the transition from coincidence rows to two-dimensional coincidence arrays in rectangular lattices as the value of c/a is varied, and the effect which this has on the relative crystal displacements which allow for the preservation of the particular coincidence pattern. In so doing, the importance of the concept of near-coincidence becomes apparent.

FORMATION OF COINCIDENCE ROWS

Rows of coincidence sites are generated in a rectangular lattice by rotating equivalent lattice vectors into one another across one of two possible mirror *lines*. In Figure 1, for example, a rotation θ_1 will bring the vector $-m'\bar{a} + n'\bar{c}$ into coincidence with the equivalent vector $m'\bar{a} + n'\bar{c}$ (a reflection across the

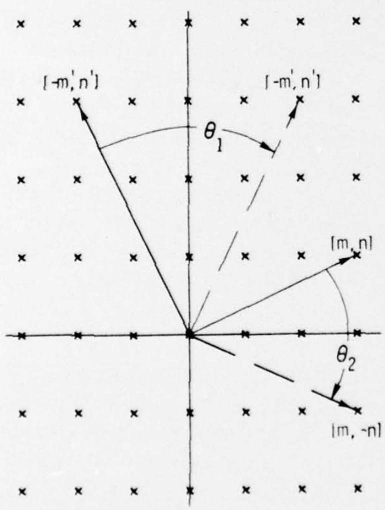

Figure 1. A general rectangular lattice. Rotations leading to the formation of typical coincidence rows are illustrated.

[0,1] mirror line), and a rotation θ_2 will bring coincidence of the vector $m\bar{a} + n\bar{c}$ with the equivalent vector $m\bar{a} - n\bar{c}$ (a reflection across the [1,0] mirror line). The angular rotation or misorientation in the first case is given by

$$\tan\theta_1/2 = m'/n'R \quad (1)$$

where R is the axial ratio c/a, and in the second case by

$$\tan\theta_2/2 = nR/m. \quad (2)$$

These relations are plotted in Figure 2 for various values of [m,n] and for values of R ranging from 0.8 to 2.0.

TWO-DIMENSIONAL COINCIDENCE ARRAYS

Intersections of the curves in Figure 2 correspond with the simultaneous formation of coincidence rows in two separate directions, and hence with the generation of a two-dimensional coincidence array in the plane of Figure 1. Under these conditions Equations 1 and 2 are simultaneously satisfied ($\theta_1 = \theta_2$) and therefore

$$m'/n'R = nR/m, \qquad (3)$$

from which follows the requirement

$$R^2 = m'm/n'n \qquad (4)$$

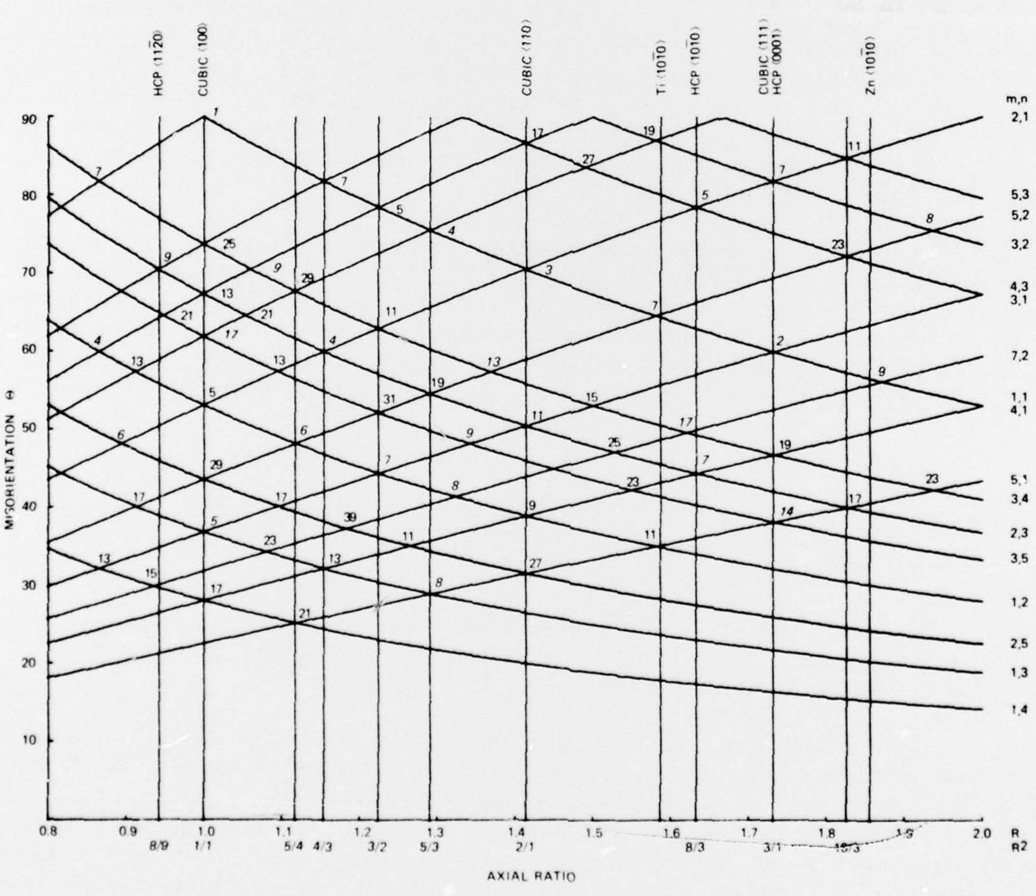

Figure 2. The misorientations generating various coincidence rows in a rectangular lattice as a function of the c/a ratio. The vectors [m,n] along which coincidence occurs are indicated. Several of the prominent intersections are labeled with the values of the planar coincidence ratio Σ_p. Rational values of $(c/a)^2$ are indicated along the abscissa along with c/a values corresponding with the rectangular superlattices on several low-index planes in cubic crystals and several hcp metals.

or R^2 must equal a rational number at the curve intersections. Several rational values of R^2 are indicated in Figure 2, corresponding with some of the prominent intersections. This represents a necessary condition for a two-dimensional CSL to exist in the plane of the two-dimensional rectangular lattice, or in three dimensions, for a three-dimensional CSL to exist in the three-dimensional crystal lattice.

In order for θ_1 to equal θ_2 the vector $[\bar{m}',n']$ must be normal to the vector $[m,n]$. It can be shown that this will be the case when

$$m' = R^2 n \qquad (5a)$$

$$n' = -m \qquad (5b)$$

Assuming that m and n have no common factors, and multiplying the calculated m' and n' by the smallest factor F which makes m' and n' both integers, the resulting vectors $[\bar{m}',n']$ and $[m,n]$ are the unit translation vectors of the two-dimensional CSL that exists at that misorientation θ in that particular rectangular lattice. The unit cell of the two-dimensional CSL will also be rectangular. This is a formalization of the procedure of Dunn and Bradhorst* as described and developed for cubic crystals by Ranganathan.[4] The three-dimensional treatment of cubic crystals has more recently been developed most formally and elegantly by Grimmer, Bollmann, and Warrington.[5]

The ratio of the area of the unit cell of the two-dimensional CSL to the area of the unit cell of the rectangular lattice will give the coincidence ratio Σ_p,[4,5] assuming that both are primitive cells containing one coincidence lattice site and one actual lattice site per cell, respectively.† In terms of the vectors $[m,n]$ and $[m',n']$, the planar coincidence ratio in the two-dimensional rectangular lattice (and hence in a single plane of a three-dimensional crystal) is

$$\Sigma_p = mn' + m'n. \qquad (6)$$

Using Equation 5 to give $[m',n']$, the planar coincidence ratio is

$$\Sigma_p = F(m^2 + n^2R^2). \qquad (7)$$

Since Σ_p is an integer, Equation 7 demonstrates once again the requirement for R^2 to be a rational number. Ranganathan presented the equivalent formula $\Sigma_p = m^2 + n^2R^2$ for coincidence-site lattices in cubic crystals.[4]

The coincidence-site lattice will always exhibit the same degree or a higher degree of symmetry than the lattice itself[1] with the result that the two-dimensional CSL will be either rectangular or centered-rectangular. Even values of Σ_p calculated from Equations 6 and 7 invariably denote the centered unit cell, examples of which are shown in Figure 3. In this latter case, the unit cell of the two-dimensional CSL defined by $[m,n]$ and $[\bar{m}',n']$ contains an additional coincidence site and so the calculated value of Σ_p must be divided by two to

4. RANGANATHAN, S. *On the Geometry of Coincidence-Site Lattices.* Acta Cryst., v. 21, 1966, p. 197-199.
5. GRIMMER, H., BOLLMANN, W., and WARRINGTON, D. H. *Coincidence-Site Lattices and Complete Pattern-Shift Lattices in Cubic Crystals.* Acta Cryst., v. A30, 1974, p. 197-207.

*C. G. Dunn and H. Bradhorst, unpublished work, 1958.

†In three dimensions the ratio of the *volumes* of the CSL unit cell to the lattice unit cell give the coincidence ratio Σ (Reference 5).

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Grain boundaries

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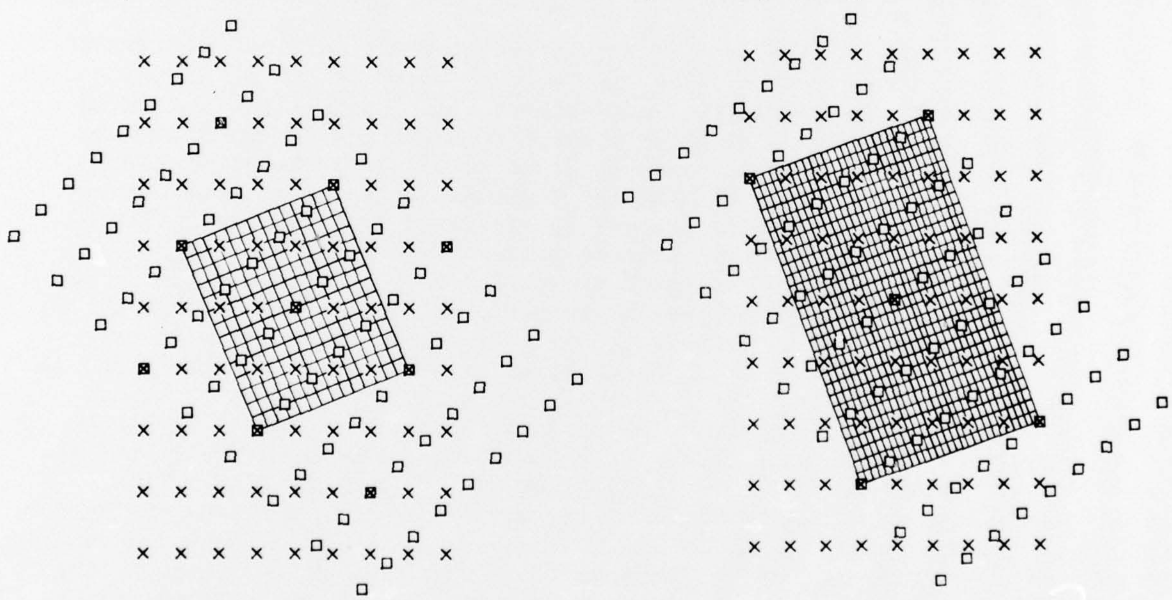
give the correct value of Σ_p. Unlike cubic crystals, where Σ_p is always an odd number,[6] an even value of Σ_p may still remain after such division in certain noncubic cases (cf. Figure 3b). Appropriate values of Σ_p are indicated for the two-dimensional CSL's represented by the intersections in Figure 2. The true Σ_p for centered-rectangular CSL's are presented in italics.*

It must be emphasized the Σ_p is the coincidence ratio only in the plane of the rectangular lattice. To obtain the coincidence ratio Σ for a three-dimensional CSL in a crystal, one must consider the coincidence that occurs in each of the uniformly stacked layers making up the crystal. Should the coincidence ratio in each layer be Σ_p, then the three-dimensional coincidence ratio is also Σ_p (i.e., $\Sigma = \Sigma_p$). This condition is frequently observed. But if coincidence in each layer is not the same (e.g., some layers often contain no coincidence sites), then Σ will be a multiple of Σ_p. It has been shown that these latter situations regularly lead to even values of Σ in crystal lattices that are not Bravais lattices (e.g., hcp crystals, Ref. 1).

A rectangular lattice can be identified on every crystallographic plane (h,k,l) in cubic crystals[5] (actually a rectangular superlattice of the real lattice in most cases). The R values for the rectangular super-lattices defined on several low-index planes have been indicated in Figure 2. Curve intersections are always associated with these values of R, corresponding with the coincidence



(a) $\Sigma_p = 7$; $(c/a)^2 = 8/3$, $\theta = 44.42^0$ (b) $\Sigma_p = 14$; $(c/a)^2 = 3/1$, $\theta = 38.21^0$

Figure 3. Two-dimensional coincidence arrays having centered-rectangular unit cells. The sublattices are the respective DSC lattices.

6. FRIEDEL, G. Lecons de Crystallographic, Paris, 1926; Blanchard, 1964 (Reprint of 1926 edition).

*Besides the extra coincidence site in centered-rectangular CSL's additional coincidence sites not taken into account by Equations 6 and 7 are sometimes obtained when the rectangular lattice is nonprimitive, further reducing the true value of Σ_p. For example, the rotation of 60° about the normal to the hcp (0001) plane or the cubic {111} plane ($R^2 = 3$) gives an actual value of $\Sigma_p = 1$ *on that one plane.*

relationship commonly reported for rotations about axes normal to these planes in cubic crystals. The Σ values are simply related to the values of Σ_p shown. R values are also indicated for the primitive rectangular lattices on <10$\bar{1}$0> planes of two hcp metals and on <10$\bar{1}$0> and <11$\bar{2}$0> planes of the hcp crystal with ideal c/a, i.e., $(c/a)^2 = 8/3$. Curve intersections occur at the R values associated with the ideal c/a, but are slightly displaced from the R values of the real metals, demonstrating that only near-coincidence is to be found in these latter cases.

PRESERVATION OF THE COINCIDENCE PATTERN

Preservation of a coincidence pattern in a grain boundary which deviates from the exact coincidence relationship requires the periodic introduction of grain boundary dislocations (GBD's) into the boundary structure. The GBD's produce relative crystal displacements (equal to the Burgers vector) that permit the coincidence pattern to be re-established in a slightly shifted location.[7] The crystal displacements which enable this to occur are given by Bollmann's DSC lattice vectors, which are simply difference vectors between real lattice sites on crystal 1 and on crystal 2 at the exact coincidence misorientation. The sub-lattices drawn in Figure 3 are the DSC lattices for those particular coincidence arrays, for example.

When the c/a ratio of the two-dimensional rectangular lattice is such that only a single row of coincidence sites occurs, the collection of difference vectors which make up the DSC lattice degenerates into a series of lines which parallel the coincidence row. In three dimensions, when only a two-dimensional CSL occurs, the DSC lattice is a series of lines parallel to the plane of the two-dimensional CSL. This implies that the component of a lattice translation parallel to the coincidence row is completely arbitrary from the standpoint of preserving this one-dimensional coincidence pattern in the two-dimensional lattice (or equivalently, from the standpoint of preserving a two-dimensional coincidence pattern in a three-dimensional crystal). However, only a small number of the infinite set of possible Burgers vectors (i.e., pattern-preserving displacements) can be of significance to a physical description of grain boundary structure. At least three factors will limit the number of physically significant pattern-preserving displacements: (i) the magnitude of the relative crystal displacements, i.e., the length of the Burgers vector of the GBD; (ii) the magnitude of the pattern shift, i.e., the dimensions of the GBD core which give the size of the boundary step between adjacent coincident regions; (iii) the fact that the Burgers vector must be normal (or nearly normal) to the boundary plane. These points have been discussed in other papers.[8,9] Suffice it to say that small values for the Burgers vector and for the pattern shift distance are favored in minimum energy boundaries, and that small pattern shift distances are possible only when c/a and θ are located *near* a curve intersection in Figure 2 (i.e., near an exact coincidence relationship).

7. BOLLMANN, W. *Crystal Defects and Crystalline Interfaces.* Springer-Verlag, New York, 1970, p. 206.
8. BRUGGEMAN, G. A., and BISHOP, G. H., Jr. *Grain Boundary Dislocations in Noncubic Crystals - I. The Model.* Army Materials and Mechanics Research Center, AMMRC TR 76-6, March 1976.
9. BRUGGEMAN, G. A., and BISHOP, G. H., Jr. *Grain Boundary Dislocations in Noncubic Crystals - II. The GBD Model Applied to Grain Boundary Facets in <10$\bar{1}$0> Tilt Boundaries in Zinc.* Army Materials and Mechanics Research Center, AMMRC TR 76-11, March 1976.

Exact coincidence rows and their corresponding two-dimensional CSL's occur in three dimensions, only in symmetric inclinations. Therefore, preservation of such patterns in boundaries in the symmetric inclination require GBD's with Burgers vectors normal to the coincidence row and hence normal to the lines of the DSC "line lattice." The Burgers vectors therefore have lengths equal to the DSC line spacing and have no component parallel to the coincidence pattern. Preservation of such an exact symmetric coincidence pattern in an asymmetric boundary, on the other hand, requires a Burgers vector component parallel to the DSC lines. As stated above, the associated pattern shift in this case will be small only when $(c/a, \theta)$ is located near an exact coincidence point in Figure 2, i.e., near-coincidence must exist. Notice too that exact asymmetric coincidence patterns exist only at exact coincidence points, so that preservation of an asymmetric coincidence pattern also is possible only when near-coincidence exists.[9] Thus, although exact two-dimensional coincidence patterns (two-dimensional CSL's) are able to occur quite generally, their significance to general boundary structures is limited unless associated with a near-coincidence relationship.

SUMMARY

The conditions for the formation of coincidence rows in rectangular lattices (and hence of two-dimensional CSL's in real crystals) have been shown to be far less restrictive than the conditions for achieving higher order coincidences. The DSC lattices degenerate into "line lattices" in cases where only one-dimensional or two-dimensional coincidence occurs in two- and three-dimensional crystals, respectively. The presence of coincidence arrays in grain boundaries of noncubic crystals is therefore not geometrically precluded, although the importance of near-coincidence and of near-CSL's remains.

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