THE STRUCTURE OF HIGH-ANGLE GRAIN BOUNDARIES*

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A coincidence model of high-angle grain boundaries can be extended to include deviations from coincidence. The generalised boundary has a terraced structure, corresponding to the densely packed planes in the coincidence lattice, and a superimposed dislocation network, corresponding to a sub-boundary in the coincidence lattice. This model is a natural extension of previous dislocation models and models based on coincidence relationships. The model explains many of the observed properties of grain boundaries and should have wide validity for the cubic system.

STRUCTURE DE JOINTS DE GRAINS A GRANDS ANGLES

Un modèle de coïncidence pour les joints de grains à grand angle peut être modifié de manière à inclure les écarts de coïncidence.

Le joint généralisé présente une structure en terrace, correspondant aux plans denses dans le réseau de coïncidence et un réseau supplémentaire de dislocations correspondant à un sous-joint dans le réseau de coïncidence.

Ce modèle est une extension naturelle des modèles de dislocations antérieurs et de modèles établis sur la base des relations de coïncidence. Il explique un grand nombre des propriétés observées des joints de grains et il semblerait valable dans de nombreux cas pour le système cubique.

DIE STRUKTUR VON GROẞWINKELKORNGRENZEN

Ein Koinzidenzmodell von Großwinkelkorngrenzen kann so erweitert werden, daß es auch Abweichungen von der Koinzidenz einschließt. Die allgemeine Korngrenze hat eine Stufenstruktur, entsprechend den dichtest gepackten Ebenen im Koinzidenzgitter, und ein überlagertes Versetzungsnetzwerk, entsprechend einer Subkorngrenze im Koinzidenzgitter. Dieses Modell ist eine natürliche Erweiterung früherer Versetzungsmodelle und von Modellen, die auf Koinzidenzbeziehungen beruhen. Das Modell erklärt viele der beobachteten Korngrenzeneigenschaften und sollte in kubischen Systemen in vielen Fällen zutreffend sein.

1. INTRODUCTION

In a previous publication[1] field-ion microscope observations of grain boundaries were reported and the observations were correlated with a model for high-angle grain boundaries based on an analysis of the coincidence relationships possible between two grains of a cubic system. In this model deviations from coincidence are regarded as being produced by a sub-boundary in the coincidence lattice coplanar with the grain boundary, in this way a high degree of coincidence can persist across a boundary whose axis of misorientation and angular misorientation do not fulfill the exact coincidence conditions.

The purpose of the present paper is to describe the previous model more fully and to examine some of the consequences and limitations of this model. The relation between the present model and previous models of the grain boundary structure will also be discussed.

2. THE MODEL

2.1 *Coincidence boundaries*

For certain specific axes and angles of misorientation two grains separated by a boundary will hold a number of lattice sites in common. Boundaries to separating grains having these special axes and angles of misorientation are known as coincidence boundaries,[2] and if the density of coincident lattice sites is high such boundaries may have unusual properties, for example a very high mobility.[3]

The simplest coincidence boundary is the twin boundary, for which the reciprocal density of common lattice points in the two grains, Σ, is 3; but coincidence boundaries exist for all odd values of Σ. Any coincidence relationship can be expressed by an axis-angle pair, and in the cubic system each such relationship can be described by 24 different axis-angle pairs, corresponding to the 24 symmetry elements of the cubic system.[4]

The reciprocal density of common lattice points, Σ, is not simply related to the reciprocal density of coincidence sites in an arbitrary boundary plane, σ. For example, in Fig. 1 it is possible to find planes for which σ is either 1, Σ or ∞. However, a boundary in a densely packed plane of the coincidence lattice must always correspond to $\sigma = 1$, while it is obvious that a boundary passing between the planes of the coincidence lattice corresponds to a coincidence site density of 0, i.e. $\sigma = \infty$. If Σ is large the most densely packed plane in the coincidence lattice is a plane of low atomic density in the real lattice, so that $\sigma = 1$ does not necessarily imply a dense packing of coincident sites. However, boundary planes corresponding to $\sigma = 1$ are expected to have the lowest

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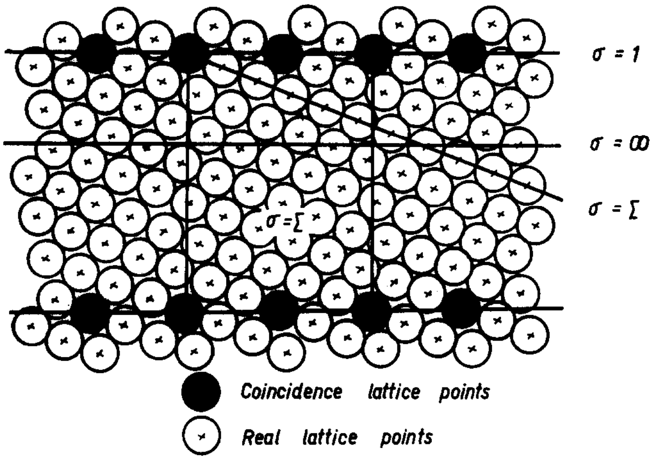


FIG. 1. Reciprocal density of common lattice points in the boundary plane, σ, as a function of the boundary orientation. The reciprocal density of lattice points in the coincidence lattice, Σ, is 19 in this example.

energy, so that boundaries running at a small angle to these planes are expected to take up a stepped structure.[1]

A fuller discussion of the conditions for and calculations of coincidence relations has been given elsewhere.[1,5]

2.2 *Step dislocations*

The step arising when a coincidence boundary makes a small angle with a densely packed plane of the coincidence lattice is effectively a small region of disorder [Fig. 2(a)]. For an arbitrary boundary orientation the steps will form a terraced structure at the boundary. Coincidence boundary migration can be thought of as a result of step migration along the boundary, and under suitable conditions multiple steps might be expected, for example as a result of a "pile-up" of steps at a precipitate particle or at a step locked by segregation.

These steps can be described in terms analogous to those used to define van der Merwe dislocations[6] at a partially coherent interface. There is no long-range strain field associated with the steps, but a step can nucleate dislocations if a suitable stress is applied to the boundary [Fig. 2(b)]. Generation of a dislocation leaves behind a strain field corresponding to a dislocation of opposite sign at the step. Repeated dislocation generation must be accompanied by simultaneous ejection of dislocations into the neighbouring grain with a corresponding increase in grain-boundary area.

2.3 *Deviation from coincidence*

It is convenient to distinguish between changes in angular misorientation and changes in axis of misorientation, although there is no significant difference in the resultant boundary structure (an angular deviation from coincidence in a relationship defined by one axis-angle pair may be equivalent to a deviation in the axis, when the same coincidence relationship is described by a different axis-angle pair). Deviations from the angular misorientation required for exact coincidence can be described by a subboundary network of dislocations superimposed on the coincidence boundary with its axis of misorientation *parallel* to the chosen axis of misorientation of the coincidence boundary. To avoid ambiguity, the Burgers vectors of the dislocations in the subboundary are defined by reference to the coincidence lattice, which is common to both grains. The subboundary dislocations will then have partial Burgers' vectors in the coincidence lattice which in general* do not correspond to unit lattice vectors in either of the two grains (Fig. 3).

Deviations in the axis of misorientation without any appreciable change in the angular misorientation can occur if the axis of misorientation of the superimposed subboundary lies *perpendicular* to the axis of misorientation of the coincidence boundary. Thus if the coincidence boundary is a pure tilt boundary containing the axis of misorientation, the subboundary will be pure twist. The coincidence boundary will then contain a superimposed network of screw dislocations.

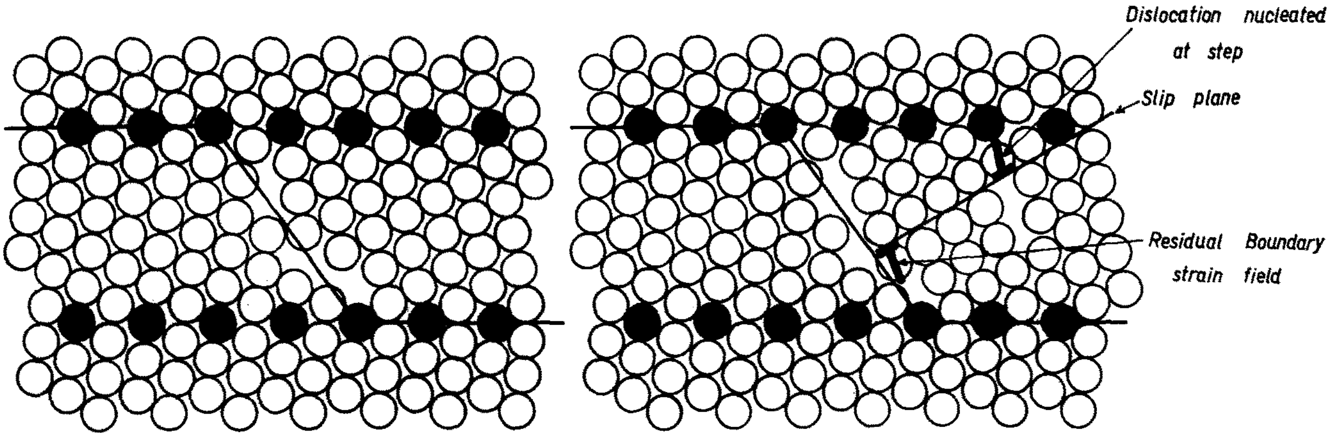
Clearly, in the general case the axis of misorientation of the sub-boundary will lie at some arbitrary angle to the axis of misorientation chosen to describe the coincidence lattice, so that deviations in both the misorientation axis and the angular misorientation will occur.

3. LIMITATIONS OF THE MODEL

3.1 *Significance of coincidence*

As pointed out previously, the most densely packed plane in the coincidence lattice is usually a plane of low atomic density in the real lattice. This is brought out by Table 1, which gives the values of Σ for the first twelve coincident lattices, the corresponding twinning directions for b.c.c. and f.c.c. crystals, the most densely packed planes in the coincidence lattice and the separation of the corresponding planes in the real lattice in terms of the separation of the close packed planes. It is clear from Table 1 that the reciprocal density of common lattice points in a boundary is not a measure of the actual degree of fit

* Dislocations in a coherent twin boundary are an exception.



(a) (b)

FIG. 2. (a) Step formation in a $\Sigma = 11$ coincidence boundary in the b.c.c. lattice (b) Generation of a dislocation at the step shown in (a).

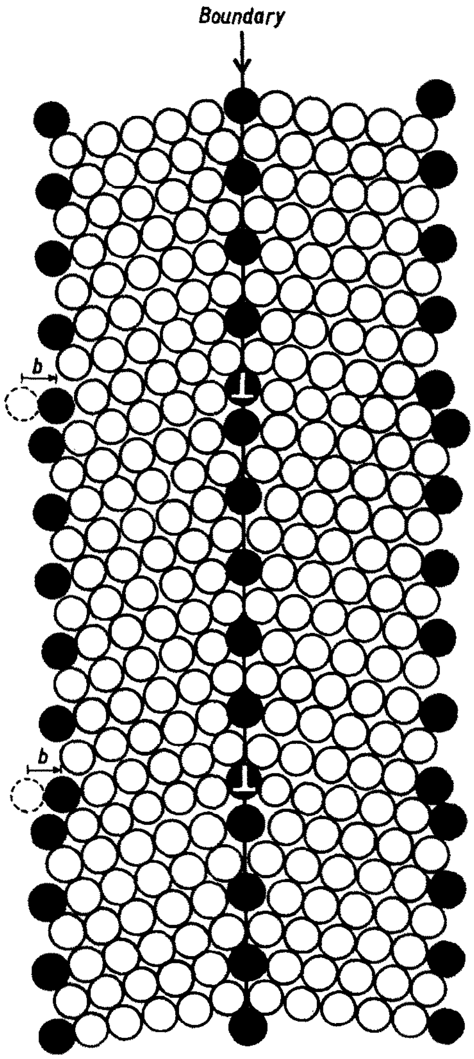


FIG. 3. Coincidence sub-boundary dislocations in the $\Sigma = 11$ boundary of Fig. 2.

TABLE 1

Σ	Twinning direction b.c.c.	Twinning direction f.c.c.	Densely packed plane b.c.c.	Densely packed plane f.c.c.	Relative separation of densely packed planes b.c.c.	Relative separation of densely packed planes f.c.c.
3	111	112	112	111	0.58	1
5	012	013	013	012	0.45	0.39
7	123	123	123	123	0.38	0.23
9	122	114	114	122	0.33	0.29
11	113	233	233	113	0.30	0.52
13a	320	510	510	320	0.28	0.24
13b	134	134	134	134	0.28	0.17
15	125	125	125	125	0.26	0.16
17a	140	350	350	140	0.24	0.21
17b	223	334	334	223	0.24	0.21
19a	133	116	116	133	0.23	0.40
19b	235	235	235	235	0.23	0.14

a,b two different coincidence lattice with the same Σ corresponding to two solutions of the equation $h^2 + k^2 + l^2 = n\Sigma$ where $n = 1$ or 2.

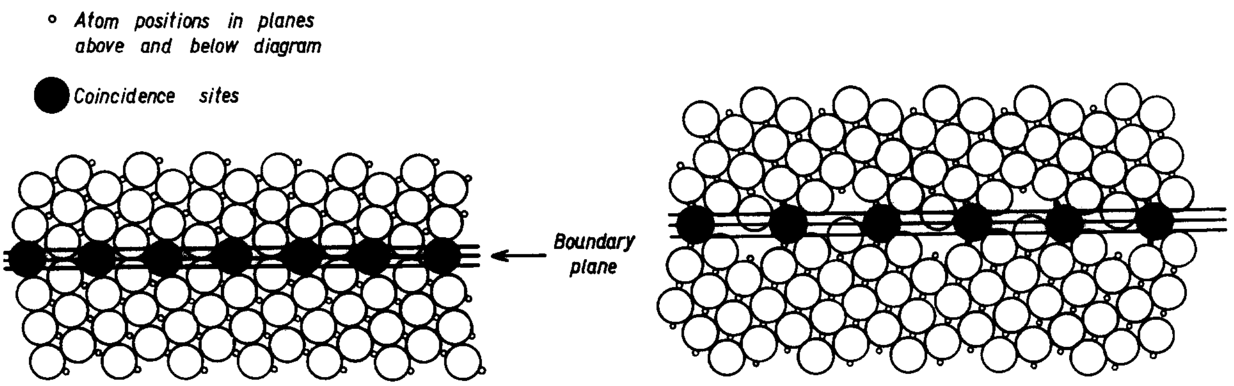
between the two lattices but refers only to the two-dimensional surface which defines the boundary. Thus in Fig. 4(a) the $\Sigma = 11$ coincidence lattice in a b.c.c. crystal generates a boundary at which the disturbance of order includes the boundary plane and the neighbouring planes in the real lattice each side of the boundary ({332} planes in this case). In the $\Sigma = 19$ coincidence lattice [Fig. 4(b)] the disturbance extends to *two* {116} lattice planes either side of the boundary. In comparing Fig. 4(a) and Fig. 4(b) it should be noted that the width of the boundary zone does not change appreciably, because the spacing of the {116} lattice planes is less than that of the {332} planes; however, Fig. 4 does illustrate the dependence of the degree of fit between the two crystals on the atomic density in the densely packed plane of the coincidence lattice. Coincidence has little significance if this density is low, i.e. if Σ is large.

3.2 *Permissible deviations from coincidence*

In the previous publication[1] it was noted that the superposition of a coincidence lattice sub-boundary on a coincidence boundary was a simple extension of the model proposed by Read and Shockley[7] for a twin boundary containing excess dislocations. It was also noted that the density of dislocations one could introduce into a coincidence boundary without destroying coincidence was limited by the density of coincident lattice at the boundary. Since the density of coincident sites decreases with increasing Σ the maximum permissible density of boundary dislocations must also decrease with Σ, so that only coincidence boundaries with small Σ will persist over any appreciable range of orientation.

The maximum permissible deviation from coincidence may reasonably be assumed to be given by an equation of the form $\theta = \theta_0(\Sigma)^{-\frac{1}{2}}$, where θ_0 is a constant, $\theta_0 \simeq 15°$. Thus for the real lattice, $\Sigma = 1$, and $\theta \simeq 15°$, corresponding to the generally accepted transition point from the dislocation sub-boundary to the high-angle grain boundary.[7]

Some idea of the range of validity of the coincidence model is given by Fig. 5, where the twinning directions corresponding to each of the 12 coincidence lattices



(a) (b)

FIG. 4. Dependence of degree of fit at low energy boundaries on Σ.
(a) Boundary in $\Sigma = 11$ coincidence lattice.
(b) Boundary in $\Sigma = 19$ coincidence lattice.

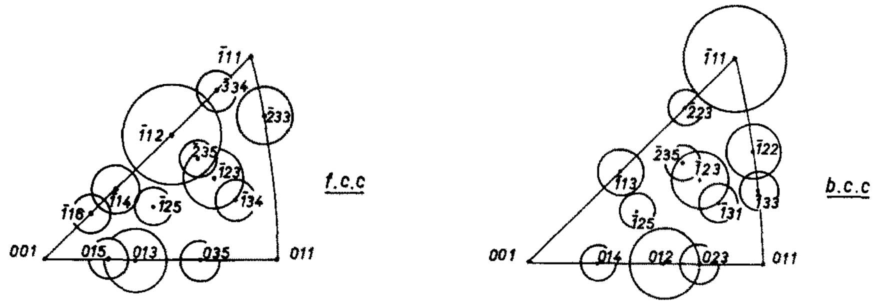


FIG. 5. Twinning systems for coincidence lattices showing estimated range of orientation over which some coincidence is maintained.

listed above have been plotted on a stereographic triangle together with the estimated maximum angular deviation from coincidence.

Limiting the number of possible coincidence lattices to 12, we can estimate the coverage given by the coincidence model. The solid angle included by the stereographic triangle is $\pi/6$ and the total angular rotation to be considered is 2π. Each coincidence lattice covers a range $4\pi[1 - \cos(\theta_0/\sqrt{\Sigma})]$ in axis of misorientation and a range $\theta_0/\sqrt{\Sigma}$ in angular deviation. Summing over the first 12 coincidence lattices and dividing by the total angular range to be covered, $\pi/6 \times 2\pi$, we find for $\theta_0 = \pi/12$ a proportional coverage of 0.42.* Clearly the coincidence lattice model should have a high degree of validity in the cubic system.

4. COMPARISON WITH OTHER MODELS

The present model of the boundary is a simple extension and combination of the model based on dense arrays of dislocations proposed by Read and Shockley[7] and the coincidence lattice model proposed by Kronberg and Wilson.[2] A grain boundary has associated with it five degrees of freedom, three that define the angle and axis of misorientation and two that define the plane of the boundary. Early models of high-angle grain boundaries assumed the structure to be independent of all five degrees of freedom.[8] The simple coincidence theory[2] brings out the dependence of the structure on the angle and axis of misorientation but ignores the two degrees of freedom associated with the plane of the boundary. In the present model the structure of a coincidence boundary depends on all five degrees of freedom. At the same time the number of axis-angle pairs describing coincidence boundaries is seen to be far greater than previously realised.

The anisotropic nature of the boundary region was postulated by Mott[9] in an attempt to explain grain boundary diffusion data, but, as in the early models,[8] Mott regarded all high-angle boundaries as structurally equivalent. Local variations in boundary structure were given a more precise meaning by Read and Shockley[7] who used a description in terms of two arrays of dislocations, a dense dislocation array (corresponding to the coincidence boundary in the present model) and a low density array (equivalent to the coincidence lattice sub-boundary in the present model). Indeed, the one significant difference in the description of the high angle boundary given here compared to that given by Read and Shockley[7] is that in the present model the concept of a dense dislocation array has been dropped in favour of the coincidence lattice description. This difference is important for three reasons:

Firstly, the ambiguity in the definition of the Burgers vector of a dislocation at a high-angle boundary is avoided by referring all such definitions to the coincidence lattice, which is common to both grains. Secondly, the difficulty in estimating the core interaction of densely packed dislocations without at the same time ignoring the structural relationship between the two grains is avoided.[10] Finally, the use of the coincidence lattice description avoids the difficulty associated with alternative descriptions of the same boundary arising from the multiplicity of axis-angle pairs generating the same coincidence lattice.

5. PREDICTIONS FROM THE MODEL

As should be clear from Section 3, the present model is *not* a general description of a high angle boundary. Indeed, one of the conclusions to be drawn from the present model is that such a description is not possible. However, the large number of axis-angle pairs describing a single coincidence lattice, taken together with the deviations from coincidence that can be accommodated by a sub-boundary dislocation network, should ensure that a high proportion of the boundaries in any polycrystalline sample can be described in terms of the

* Suiter (private communication) has pointed out that this is an overestimate, since it includes some coverage in neighbouring triangles.

present model. This proportion should be higher than would be calculated on the basis of random nucleation, both because nucleation is seldom random and because boundaries falling outside the range of validity of the model should have, on average, significantly lower mobilities[3] and higher energies.[7]

A boundary based on the present model has the following characteristics:

(a) Its axis and angle of misorientation lie within a few degrees of a coincidence relationship.
(b) It contains a step structure dependent on the angle between the boundary plane and the densely packed planes of the coincidence lattice.
(c) It has superimposed upon it a dislocation network constituting a subboundary in the coincidence lattice.

As corollaries of these characteristics:

(i) The boundary is anisotropic, regions of disorder alternating with regions of coincidence.
(ii) The boundary is non-planar, but contains steps which are disordered regions.
(iii) There is an elastic strain-field associated with the boundary arising from the presence of the dislocation network.

It should be noted that the presence of ledges[11,12] and dislocations[13] at the boundary arises naturally out of the model and is not arbitrarily introduced to account for experimental observations. Also nothing has been said about the energy of the boundary, which must depend on structure, but can only be deduced approximately.[7,10]

The variations in boundary structure predicted by the present model are expected to show up in those properties which are strongly structure sensitive: segregation to the boundary,[3] grain boundary diffusion,[14] and grain boundary migration[3] are all known to depend on the boundary structure; dislocation generation at a boundary[15] and slip propagation across a boundary[16] also exhibit considerable structure dependence.

6. CONCLUSIONS

A description has been given of a model for high-angle grain boundaries based on an extension and combination of the coincidence lattice model of Kronberg and Wilson[2] and the dislocation model of Read and Shockley.[9] The range of validity of the model and the characteristics and properties of grain boundaries falling within this range of validity have been described.

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