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Grain Boundary Parameters

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The specification of the boundary between adjacent crystals of the same solid is discussed. It is shown that for planar boundaries the minimum number of parameters required is nine. A convenient choice of the grain boundary parameters is indicated, and their effect on the boundary structure exemplified.

1. Introduction

The specification of a grain boundary is a basic question when discussing the structure and properties of grain boundaries in crystalline solids. In general, the relative orientation of the two adjacent crystals is given in terms of an axis/angle pair, and, for planar boundaries, the orientation of the plane of the boundary is also specified. This involves giving the values of 5 parameters, 3 to specify the relative orientation of the two crystals and 2 to indicate the plane of the boundary. However, a description in terms of 5 parameters is not complete, and it will be shown in the present paper that more parameters have to be introduced in order to completely characterize a grain boundary.

2. The relative orientation of the two crystals

We take two crystals in an arbitrary orientation, and consider the problem of specifying the relative orientation of their identical space lattices A and B. Each lattice may be regarded as a 'solid' and we take lattice A as the reference 'solid'. Then lattice B has 6 degrees of freedom, as any solid has. The 6 parameters required to specify the relative orientation of A and B may be chosen in a variety of ways. A particularly convenient choice is the following. The actual configuration of lattice B can be obtained from lattice A by the product of a rotation and translation of A. The rotation can always be chosen so that the axis of rotation $\mathbf{w}$ contains a lattice point P_A of lattice A. We thus need two parameters to specify the axis and another which is the angle of rotation θ. Finally the translation $\mathbf{t}$ which brings the rotated A lattice (A_r) in coincidence with B, is determined by 3 parameters, for instance the 3 components of $\mathbf{t}$ parallel to the crystal axes of A (or A_r).

A particular bicrystal will then be specified as follows: $(\mathbf{w},\theta,\mathbf{t})$ with the convention that $\mathbf{w}$ contains a lattice point P_A of A. The translation $\mathbf{t}$ is not, in general, taken into account in the various grain-boundary models (Brandon, Ralph, Ranganathan & Wald, 1964; Brandon, 1966; Bishop & Chalmers, 1968), but it has an appreciable effect on the atomic configuration at the grain boundary. Fig. 1 shows, in a two dimensional representation, the effect of $\mathbf{t}$ on the grain boundary structure. The axis $\mathbf{w}$, normal to the plane of the Figure, contains the lattice point P_A and $\theta=53{\cdot}1°$ ($\text{tg}\,\theta=\frac{4}{3}$). In Fig. 1(*a*) the translation is zero ($\mathbf{t}=0$) and there is partial coincidence of lattice points. In Fig. 1(*b*), $\mathbf{t}\neq 0$ and no coincidence occurs.

Since each lattice is invariant to a translation by a lattice vector, the axis $\mathbf{w}$ may be chosen to contain a given lattice point. The translation $\mathbf{t}$ will in general change as the lattice point P_A is replaced by another lattice vector of A and a lattice vector of A_r. In some applications it may be convenient to choose the shortest vector $\mathbf{t}$ to describe the relative orientation of the two crystals. This will be the vector between the pair of lattice points, P_A and P_B, one in each lattice, which are closest to each other. The axis of rotation will then contain the lattice point P_A of this pair. In some cases, however, this point P_A can be very far from the actual, finite boundary between the two crystals. It may then be more convenient to take the axis of rotation closer to the grain boundary and use the appropriate translation $\mathbf{t}$ to define the relative orientation. It may also happen that the relative orientation is such that it can be described using a $\mathbf{t}$ as small as one wants, but not equal to zero; in this case an axis of misorientation near the boundary region is again a convenient choice.

If the two lattices are related by a pure rotation, *i.e.* if $\mathbf{t}=0$ (or equivalent to zero) they have at least a common lattice point. Conversely, if the two lattices have a common point, they can always be specified in such a way that $\mathbf{t}=0$.

If $\mathbf{t}$ is perpendicular to $\mathbf{w}$, the relative orientation $(\mathbf{w},\theta,\mathbf{t})$ of the two lattices can always be described by a pure rotation $(\mathbf{w}',\theta)$ with the same angle θ, but the axis $\mathbf{w}'$, parallel to $\mathbf{w}$, will not, in general, contain a lattice point (unless $\mathbf{t}$ is equivalent to zero). For instance, in Fig. 1(*b*), where $\mathbf{t}$ is perpendicular to $\mathbf{w}$, the axis $\mathbf{w}'$ contains the point P'. In what follows we shall always adhere to the convention that the axis of rotation contains a lattice point.

When the lattice admits symmetry rotations, there will be as many equivalent axis/angle pairs for a given bicrystal as symmetry rotations of the lattice. In this case it may be convenient to choose the axis/angle pair that involves the smallest angle. In bicrystals

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with cubic lattices there are 24 equivalent axis/angle pairs and the smallest angle θ is always smaller than 62°48′ (Goux, 1961). It should be noted that **t** is not affected when the axis/angle pair is replaced by an equivalent one.

3. The specification of the boundary region

We shall now suppose that the two crystal lattices have a certain specific orientation, given by the 6 parameters $(\mathbf{w}, \theta, \mathbf{t})$, and consider the problem of defining the transition region between the two crystals, *i.e.* the grain boundary. The problem is more delicate than the one of specifying the relative orientation of the crystals, and different approaches are possible.

Firstly, we shall use a simplified model for a grain boundary, assuming that the width of the boundary region is zero, so that on each side of the boundary surface the lattice points of the crystals A and B, respectively, are unperturbed (there may, eventually, be lattice points on the boundary surface). Let us consider, first, the case where the boundary surface is planar. The orientation of the plane of the boundary (or of its normal) is defined by two parameters. But it is also necessary to define the location of the plane relative to the two lattices A and B, since the atomic pattern at the boundary will, in general, be affected by a translation of the boundary plane (see example in Fig. 2). This means that a further parameter is required, for instance the distance of the plane to the lattice point P_A referred to in the previous section. When the boundary is curved, the specification of the boundary surface will require 6 parameters so that the number of degrees of freedom will be 12.

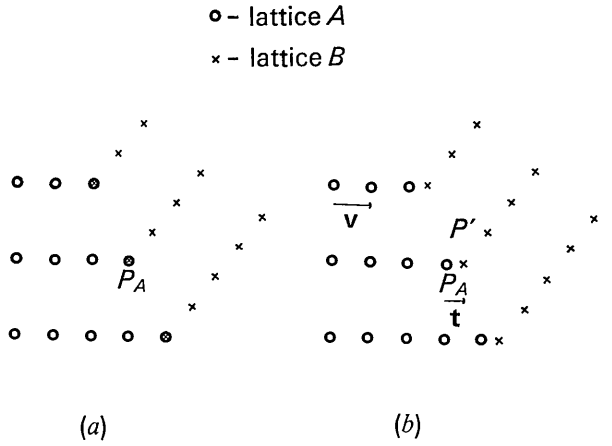

Fig. 1. Two differently oriented bicrystals AB. The axis of rotation is in both cases normal to the plane of the diagram and contains the lattice point P_A. The angle of rotation is $\theta = 53{\cdot}1°$. In (*a*) the translation $\mathbf{t}=0$, while in (*b*) $\mathbf{t}=\frac{1}{2}\,\mathbf{v}$, where **v** is the lattice vector of A indicated in the Figure. In (*b*) the relative orientation of the two lattices could as well be described as a pure rotation, with the same θ, and axis containing P'.

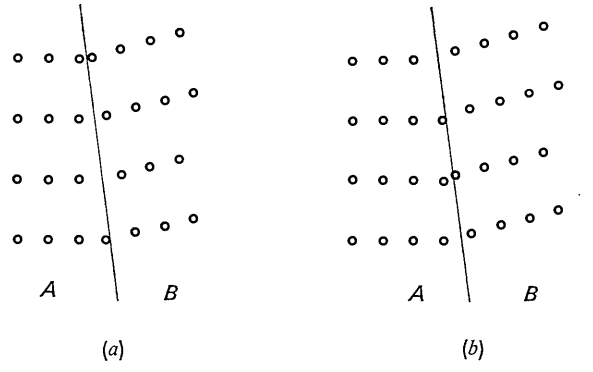

Fig. 2. Two-dimensional model of a planar boundary between two lattices A and B showing the alteration of the pattern at the boundary upon translation of the boundary plane. The relative orientation of the two lattices is the same in (*a*) and (*b*).

Actual grain boundaries in solids have widths of the order of 2–3 atom diameters and in the boundary region the atom sites will be more or less perturbed. Consequently, the concept of a boundary plane (or surface) is not strictly applicable. The difficulty can be overcome by introducing a definition of 'unperturbed' atom, as the one which occupies a position in the crystal within a certain small distance from its site in the perfect lattice. It would then be possible to define two surfaces limiting the boundary region, each containing the sites, closer to the boundary, of the unperturbed atoms of the two crystals. In this context the number of grain-boundary parameters would be quite large, and the specification of a grain boundary would become a complicated question. The situation can be simplified by indicating the 'average grain boundary surface', *i.e.* a surface lying between the two previously defined surfaces.

4. Discussion

The atomic structure and properties of a grain boundary depend, in general, on a large number of parameters. In the simplest case of a planar boundary nine parameters are required to characterize the boundary. The relative orientation of the crystals is always specified by 6 parameters, while 3 or more are required to define the orientation and location of the transition region between the two crystals.

Special grain boundaries such as coincidence lattice site (c.s.l.) boundaries (Ranganathan, 1966) and grain boundaries with a periodic pattern of atoms, may occur for particular values of the parameters, but the conditions to be satisfied are so stringent that such boundaries will be very rare, even in cubic lattices. It has been argued (*e.g.* Bishop & Chalmers, 1968) that small deviations from the correct parameters for a special grain boundary will only slightly affect the special properties of the boundary (*e.g.* low energy, high mobility). However, these deviations are not in general precisely defined and, as a rule, only the effect of a change in the axis/angle pair and orientation of

the plane of the boundary are considered. In particular the effect of **t** on the structure of a grain boundary is ignored, or at least not explicitly considered. For instance, for a bicrystal to be in a c.s.l. orientation it is necessary that $\mathbf{t}=0$. This is implied by the existence of common lattice points (*cf.* §2). Even when the axis/angle pair has the correct values for the existence of a c.s.l., it is necessary that $\mathbf{t}=0$ for a c.s.l. boundary to occur. Fig. 1 shows how the parameter **t** can profoundly change the atomic configuration at the boundary.

The necessity of so many parameters to characterize a grain boundary, together with the fact that small fluctuations of the boundary parameters may drastically affect the properties of grain boundaries, make the experimental determination of the parameters a difficult and important question. The methods generally employed (diffraction techniques) do not provide complete information on the relative orientation of the two crystals and on the location of the boundary. They only give the direction of the axis of misorientation and the value of θ, while **t** remains undetermined. Field-ion microscopy is probably unique in providing complete information on the grain boundary parameters (*cf.* Fortes & Smith, 1970).

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Acta Cryst. (1972). A**28**, 102

The Theory of X-ray Crystal Diffraction for Finite Polyhedral Crystals. I. The Laue–Bragg Cases

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The entrance and exit surfaces are defined with respect to the Poynting vector, and the Bragg and Laue cases are redefined separately with respect to the wave vector on the entrance and exit surfaces. In this paper, the diffraction phenomena in the Laue (on the entrance surface)–Bragg (on the exit surface) case are discussed on the basis of both the plane-wave and spherical-wave theories. The two-beam approximation is used throughout, by taking account of absorption. Total reflexion is expected on the exit surface inside the crystal for either direct or Bragg-reflected waves. The wave fields in the spherical-wave theory are represented by Bessel functions, in the forms which are very similar to the Laue case (Kato, *J. Appl. Phys.* (1968). **39**, 2225). This implies that the reflected waves are regarded as a divergent cylindrical wave starting from an imaginary focal point. The treatments described here are easily extended to more general cases in plane-bounded crystals. In this sense, this paper is a preparation for treating the diffraction phenomena in a finite polyhedral crystal.

Introduction

The phenomena of Pendellösung in crystal diffraction were originally predicted by Ewald (1916) and observed first by Kato & Lang (1959) in the X-ray case. Kato (1961*a*,*b*) has interpreted theoretically the observed fringe pattern by regarding the incident wave as a spherical wave. This theory is called 'spherical-wave theory' and the corrcsponding wave fields are called 'spherical-wave solutions'. The conventional theory in which the incident wave is regarded as a plane wave is called 'plane-wave theory' and the corresponding wave fields called 'plane-wave solutions'. Later, Kato, Usami & Katagawa (1967) extended the spherical-wave theory to the case of the crystal including a stacking fault.

In the above theories, although the exit surface is not necessarily parallel to the entrance surface, it is assumed that both *O* (direct) and *G* (Bragg-reflected) waves pass through the exit surface. In general cases, however, one of the *O* and *G* waves cannot pass through the exit surface when it is nearly parallel to the lattice plane concerned. In fact, Borrmann, Hildebrandt & Wagner (1955), Borrmann & Lehmann (1963) and Lehmann & Borrmann (1967) have studied experimentally diffraction phenomena under this condition. They have also considered the plane-wave theory for a special geometry* and highly absorbing crystals.

* A symmetrical Laue case in which the lattice plane is perpendicular to the entrance surface and parallel to the exit surface.