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Tilt and Twist Boundaries

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Tilt and twist components are determined for cubic bicrystals meeting at a planar boundary. It is shown that any boundary is nearly either a twist or tilt boundary, but the distinction between the two types is, in some cases, ambiguous.

Introduction

In the study of the structure and properties of grain boundaries in solids it is useful to consider the special cases of pure tilt and pure twist boundaries (*e.g.* Read & Shockley, 1950; Read, 1953; Bishop & Chalmers, 1971; Weins, Gleiter & Chalmers, 1971). The relative orientation of the space lattices, A and B, of two crystals meeting at a grain boundary can be described as the product of a rotation $(\mathbf{u},\theta)$ and translation $\mathbf{t}$, with the convention that the axis of rotation, $\mathbf{u}$, contains a lattice point of lattice A (Fortes, 1972). Let $\mathbf{n}$ be the normal to the plane of the boundary. Then, if $\mathbf{u}$ is parallel to $\mathbf{n}$ the boundary is a (pure) twist boundary; it is a (pure) tilt boundary when $\mathbf{u}$ is normal to $\mathbf{n}$, *i.e.* when the axis of misorientation is parallel to the boundary plane. The structural differences between these two types of boundary are particularly noticeable in the case of low-angle boundaries; these can be described in terms of edge or screw dislocations respectively, depending on whether the boundary is a tilt or twist boundary (*e.g.* Read, 1953).

The classification of a planar grain boundary as a tilt or twist boundary can, in some cases, be ambiguous. In triclinic bicrystals, the axis/angle pair $(\mathbf{u},\theta)$ describing the relative orientation is unique and no ambiguity arises in the definition of tilt or twist boundaries. In all other cases the situation is more complex. For instance, the misorientation of two cubic lattices can be described in 24 different ways (Goux, 1961) and cases may occur, as we will show, where a grain boundary may be classified both as a tilt and twist boundary.

Tilt and twist components in cubic bicrystals

A planar grain boundary between two crystals will in general be a mixed boundary, which can be described as the combination, or product, of tilt and twist components. We now derive, for the case of cubic crystals, this description in terms of tilt and twist components, and discuss the complications that result from the non-uniqueness of the axis/angle pair. Let A and B be the adjacent grains and u_1,u_2,u_3, the direction cosines of the axis of misorientation, $\mathbf{u}$, relative to the cube axes of the unit cell; the u_i are the same in the two crystals and proportional to the Miller indices of the direction $\mathbf{u}$. A clockwise rotation ($0<\theta\le 180°$) of lattice A, followed by a translation $\mathbf{t}$ brings it in coincidence with B. The unit normal $\mathbf{n}$ to the plane of the boundary has components $n_1n_2n_3$ relative to the cube axes of A. At this stage the n_i are defined except for their signs.

The product of two clockwise rotations $(\mathbf{n},\nu)$ and $(\mathbf{l},\lambda)$ of a rigid body (in this order, and with the axes referred to the same reference system) is equivalent to a simple rotation $(\mathbf{u},\theta)$ defined by

$$\cos\frac{\theta}{2}=\cos\frac{\nu}{2}\,.\,\cos\frac{\lambda}{2}-\sin\frac{\nu}{2}\,.\,\sin\frac{\lambda}{2}\,.\,(\mathbf{n}\,.\,\mathbf{l}) \tag{1}$$

$$\frac{\sin\frac{\theta}{2}}{\sin\frac{\nu}{2}\,\sin\frac{\lambda}{2}}\,\mathbf{u}=-(\mathbf{n}\wedge\mathbf{l})+\mathbf{n}\,\mathrm{ctg}\,\frac{\lambda}{2}+\mathbf{l}\,\mathrm{ctg}\,\frac{\nu}{2} \tag{2}$$

where $(\mathbf{n}\,.\,\mathbf{l})$ and $(\mathbf{n}\wedge\mathbf{l})$ are scalar and vector products, respectively. This result is easily obtained by considering the rotation matrices N, L and U, related by

$$\mathsf{U}=\mathsf{L}\,.\,\mathsf{N}\,. \tag{3}$$

Using equations (1) and (2), and referring all rotation axes to the cube axes of A, we obtain the following results for the decomposition of $(\mathbf{u},\theta)$ in twist, $(\mathbf{n},\nu)$, and tilt, $(\mathbf{l},\lambda)$, components:

(*a*) angle of twist, ν:

$$\mathrm{tg}\,\frac{\nu}{2}=\mathrm{tg}\,\frac{\theta}{2}\,.\,(\mathbf{u}\,.\,\mathbf{n})\,. \tag{4}$$

The sense of $\mathbf{n}$ is chosen in such a way that $0<\nu\le 180°$.

(*b*) angle of tilt, λ:

$$\cos\frac{\lambda}{2}=\frac{\cos\frac{\theta}{2}}{\cos\frac{\nu}{2}}\,; \tag{5}$$

(*c*) the tilt axis, $\mathbf{l}$, is obtained from

$$\begin{aligned}&\mathbf{l}\,.\,\mathbf{n}=0\\&\mathbf{l}\,.\,\mathbf{l}=1\\&\mathbf{l}\,.\,\mathbf{u}=\mathrm{tg}\,\frac{\lambda}{2}\,.\,\mathrm{ctg}\,\frac{\theta}{2}\,.\end{aligned} \tag{6}$$

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When $\theta = 180°$, equations 4 and 5 cannot be applied. The solution in this case is as follows: if $\mathbf{u}\,.\,\mathbf{n} \neq 0$, $\nu = 180°$ and $\cos \lambda/2 = \mathbf{u}\,.\,\mathbf{n}$; if $\mathbf{u}\,.\,\mathbf{n} = 0$, the boundary is pure tilt ($\lambda = 180°$; $\nu = 0$).

If the tilt rotation is applied before the twist, the angles ν and λ are the same, and the axis of tilt $\mathbf{l}'$, is obtained from $\mathbf{l}$ by rotation $(\mathbf{u}, \theta)$. We may therefore conclude that the tilt and twist angles are the same whatever the order of the two rotations.

If we now multiply the rotation $(\mathbf{u}, \theta)$ by any of the 23 symmetry rotations $(\mathbf{s}, \sigma)$ of the cubic lattice we obtain equivalent descriptions $(\mathbf{u}', \theta')$ for the relative orientation of the two lattices. The symmetry rotations will be performed on lattice B, after the rotation $(\mathbf{u}, \theta)$, and we shall refer $\mathbf{s}$ to the cube axes of B (*i.e.* $\mathbf{s}$ is a unit vector in the directions [001], [011] or [111] of lattice B). It can be shown that the new rotation matrix U' is related to U by

$$\mathsf{U}' = \mathsf{U}\,.\,\mathsf{S} \tag{7}$$

where S is the matrix representing the rotation $(\mathbf{s}, \sigma)$, referred to the cube axes of B. Each of the equivalent rotations can now be decomposed into tilt and twist components, in the same way as was done for the original rotation. The angle of twist, ν', for each equivalent description is given by

$$\operatorname{tg}\frac{\nu'}{2} = \frac{-(\mathbf{u}\wedge\mathbf{n})\,.\,\mathbf{s} + (\mathbf{n}\,.\,\mathbf{s})\,.\,\operatorname{ctg}\frac{\theta}{2} + (\mathbf{u}\,.\,\mathbf{n})\,.\,\operatorname{ctg}\frac{\sigma}{2}}{\operatorname{ctg}\frac{\theta}{2}\,.\,\operatorname{ctg}\frac{\sigma}{2} - \mathbf{u}\,.\,\mathbf{s}} \tag{8}$$

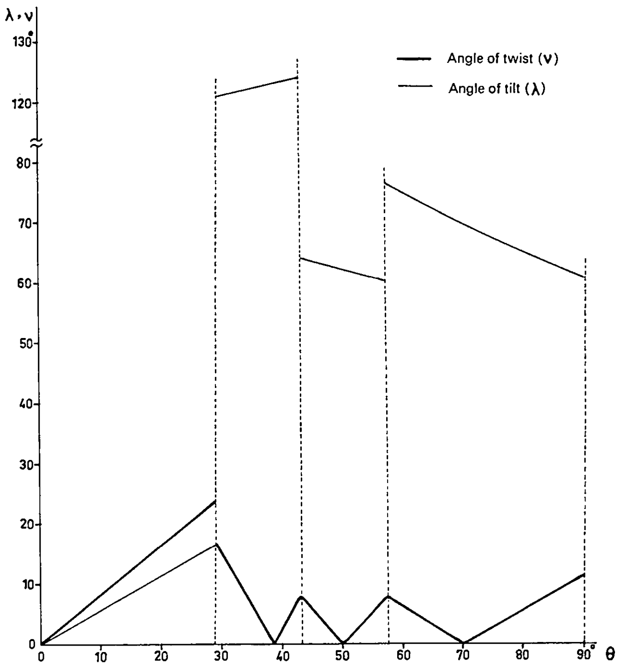

Fig. 1. The lower curve gives the smallest angle of tilt or twist for a grain boundary parallel to $(111)_A$ between two cubic crystals A and B, with a misorientation θ about [011]. The upper curves give the corresponding angle of twist or tilt.

and the associated angle of tilt, λ', is obtained from

$$\cos\frac{\lambda'}{2} = \frac{\cos\frac{\theta}{2}\,.\,\cos\frac{\sigma}{2} - \sin\frac{\theta}{2}\,.\,\sin\frac{\sigma}{2}\,.\,(\mathbf{u}\,.\,\mathbf{s})}{\cos\frac{\nu'}{2}} \tag{9}$$

Description of the grain boundary

A boundary can be classified as a pure-tilt boundary if, for any $(\mathbf{s}, \sigma)$, we have $\nu' = 0$; and as a pure-twist if $\lambda' = 0$. We note that for a given axis of misorientation of two cubic crystals there are, in general, 24 orientations for the plane of the boundary which correspond to a pure-twist boundary. It may happen that a grain boundary is simultaneously a pure-tilt and pure-twist boundary. In fact, suppose that in the original description $\mathbf{u}$ is parallel to $\mathbf{n}$, so that the grain boundary can be classified as a pure-twist boundary. For it to be a pure-tilt boundary as well there must be an equivalent $\mathbf{u}'$ such that $\mathbf{u}'\,.\,\mathbf{n} = 0$ or $\mathbf{u}'\,.\,\mathbf{u} = 0$. This condition is satisfied provided there is a $(\mathbf{s}, \sigma)$ such that

$$\operatorname{tg}\frac{\theta}{2} = -(\mathbf{u}\,.\,\mathbf{s})\,.\,\operatorname{tg}\frac{\sigma}{2}\,. \tag{10}$$

The angle of tilt is then given by

$$\cos\frac{\lambda'}{2} = \frac{\cos\frac{\sigma}{2}}{\cos\frac{\theta}{2}}\,. \tag{11}$$

It can be shown that the smallest angle of misorientation for which a boundary is both tilt and twist is 65·6° ($\cos\theta = \sqrt{2} - 1$). The normal $\mathbf{n}$ to the plane of the boundary has one of its direction cosines equal to $(\sqrt{2} - 1)^{1/2}$. A 65·6° rotation about $\mathbf{n}$ is equivalent to a 65·6° rotation about an axis normal to $\mathbf{n}$.

A small-angle boundary can be described as a unique product of small twist and small tilt components. Consequently, there is no ambiguity in the dislocation model of low-angle boundaries. However, for high-angle boundaries, it is in general not possible to associate each type of dislocation with each type of boundary. This fact may be important in a discussion of grain boundary dislocations in high-angle boundaries.

For a given grain boundary one may always choose the description involving the smallest angle of tilt or twist, so as to make the boundary, as nearly as possible, a pure-twist or a pure-tilt boundary. For example, a given grain boundary may involve in one description a 3° tilt component, and in another description, a 7° twist component. We would then say that the boundary is almost (within 3°) a pure-twist boundary, and choose this description for the grain boundary. In fact, any planar grain boundary between two cubic crystals is almost either a pure-tilt or pure-twist boundary. To illustrate this point we consider a grain boundary parallel to $(111)_A$ between two cubic crystals A and B with a misorientation θ about [011]. Since the axis of misorientation is a twofold axis of symmetry, rotations of angles θ and $(180° - \theta)$ are equivalent. Fig. 1 shows, for each value of θ $(0 < \theta \leq 90°)$, the angles of tilt and twist which correspond to the equivalent description involving the smallest angle of tilt or twist. The maximum deviation from a pure case is 16·9° and occurs for $\theta = 29{\cdot}5°$. Pure-tilt boundaries occur for the following values of θ: 39·0, 50·5 and 70·5°.

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The Coupling of the Thermal Motions of the Atoms in a Crystal as Deduced from the Acoustic Spectrum of the Thermal Diffuse Scattering

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The strength of the coupling of the motions of the atoms in different cells of a crystal is investigated by means of the acoustic spectrum of the thermal diffuse scattering. The calculations are performed for a monatomic cubic crystal. Correlation coefficients, which express the amount of in-phase motions of remote atoms in the crystal, are approximately determined from the term $1/q^2$ of the acoustic spectrum. This term is valid for all crystals. We find that the coupling of the motions of the atoms is approximately inversely proportional to the distance between the atoms in the crystal.

1. Introduction

In the usual lattice-dynamical treatment of the thermal motions of the atoms it is assumed that there are forces among the atoms in the crystal so that the motions of the atoms are coupled. This assumption means that the internal motions of a lattice can be represented by a superposition of separate running or standing waves (in the harmonic approximation). In such a wave all atoms move with the same frequency and a phase shift which is determined by the wavelength and the position of the atom in the crystal. Hence, for such a wave a coupling of the motions of even widely separated atoms in the crystal exists. In a crystal with many cells there are as many waves which are excited according to the laws of quantum statistics. Because of the different wavelengths the superposition of the waves in the motions of any particular atom prevents a noticeable effect of thermal coupling between widely separated atoms in the crystal. This means that in the crystal two atoms show a noticeable in-phase (or out-of-phase) motion only within a certain distance. Now we want to know how large this distance is, or to what extent the coupling of the motions of the atoms decreases with increasing distance.

The interatomic thermal coupling becomes manifest in the acoustic spectrum of the thermal diffuse scattering, which shows sharp maxima at the reciprocal-lattice points. Thus it should be possible to draw conclusions about the strength of the interatomic coupling from the profile of the acoustic spectrum. Such an attempt will be made in this paper. We restrict our treatment to a monatomic cubic crystal and only discuss the manifest acoustic spectrum of the first order.

2. Derivation of the coupling terms

The intensity of the first-order acoustic spectrum for a monatomic cubic lattice is given by

$$I(\mathbf{S}/\lambda) = f_0^2\, e^{-2M} \sum_{\mathbf{n}} \sum_{\mathbf{m}} \sum_{\mathbf{q}j} G_{\mathbf{q}j} \exp\{2\pi i\, \mathbf{S}/\lambda \times (\mathbf{r_n} - \mathbf{r_m})\} \cos\{\mathbf{q} \cdot (\mathbf{r_n} - \mathbf{r_m})\}\,, \quad (1)$$

where

$$\sum_{\mathbf{q}j} G_{\mathbf{q}j} = 2M\,; \quad (2)$$

and for temperatures well above the Debye temperature

$$G_{\mathbf{q}j} = \frac{k_B T}{mN\omega_j^2(\mathbf{q})} \left[\frac{2\pi}{\lambda}\, \mathbf{S} \cdot \mathbf{e}(\mathbf{q}j)\right]^2, \quad (3)$$

(*cf.* James, 1948, equations 5·27, 5·23 and 5·25). The symbols have the following meaning:

λ = wavelength of the X-rays,
$\mathbf{S}/\lambda$ = vector in reciprocal space, $S = |\mathbf{S}| = 2 \sin \theta$,
f_0 = scattering factor for the atom at rest,
$\mathbf{n}, \mathbf{m}$ = indices to denote the cell in the crystal; the components n_i and m_i are integer,