density as represented by a Fourier series with the observed structure factors as coefficients. This is a very interesting result, but it should be noted that the criterion for atomic position (maximum of electron density) is different from that of obtaining a least-squares fit for the entire electron density map, and that different weighting is required for atoms of differing atomic number. One would expect the least-squares fit to give a better estimate of the atomic positions, but in some applications it could be that the position of the maximum electron density is the focus of interest. Cruickshank (1952) has obtained results similar to Cochran's for the relation between peaks in a Patterson synthesis and refinement in a suitably weighted R_2.

These reflexions were stimulated by the problem of locating the halogen atoms in Cd analogues of apatite (Sudarsanan, Wilson & Young, 1972; a full account is in preparation). I am indebted to Professor R. A. Young for stimulating discussions and to Professor D. W. J. Cruickshank, Dr David Harker and Professor M. M. Woolfson for helpful correspondence. Travel and subsistence expenses provided by The Royal Society and The William Waldorf Astor Foundation made possible a visit to Atlanta during which the work was completed.

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Coincidence-Site Lattices

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The possibility that two arbitrary lattices, 1 and 2, have a coincidence-site lattice (CSL) in common is examined. Let **T** be the 3×3 matrix that maps a basis of lattice 1 onto a basis of lattice 2 and let $\|\mathbf{T}\|$ be the absolute value of its determinant. It may be assumed that $\|\mathbf{T}\|\geq 1$. There is a CSL if, and only if, **T** is rational. The main result is that the density ratio, Σ_2, of coincidence points to points of lattice 2 is equal to the least positive integer n such that $n\mathbf{T}$ and $n\|\mathbf{T}\|\mathbf{T}^{-1}$ are integral matrices. A basis for the CSL can be determined quickly if lattices 1 and 2 are related by a rotation.

Density of coincidence sites

The coincidence-site lattice model of a grain boundary considers the lattices that correspond to the crystals on both sides of the boundary (for example see Brandon, Ralph, Ranganathan & Wald, 1964). Working with this model we have to find out whether the metric properties of the lattices and their observed relative orientation are such that the two lattices, which we shall call 1 and 2, have vectors in common. If there are common vectors, they will form either a linear, a planar, or a spatial lattice. In the last case we shall speak of a coincidence-site lattice (CSL) and shall denote by Σ_1 (or Σ_2) the ratio of the volumes of primitive cells for the CSL and for lattice 1 (or 2). Σ_1 and Σ_2 are positive integers. Let the vectors $\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3$ form a basis of lattice 1 (*i.e.* $\mathbf{b}_1,\mathbf{b}_2$, and $\mathbf{b}_3$ span a primitive cell of lattice 1) and let $\mathbf{b}'_1,\mathbf{b}'_2,\mathbf{b}'_3$ be a basis of lattice 2. We can write

$$\begin{aligned}\mathbf{b}'_1&=t_{11}\mathbf{b}_1+t_{12}\mathbf{b}_2+t_{13}\mathbf{b}_3\\ \mathbf{b}'_2&=t_{21}\mathbf{b}_1+t_{22}\mathbf{b}_2+t_{23}\mathbf{b}_3\\ \mathbf{b}'_3&=t_{31}\mathbf{b}_1+t_{32}\mathbf{b}_2+t_{33}\mathbf{b}_3\,,\end{aligned}$$

or, introducing matrix notation,

$$b'=\mathbf{T}b,$$

where

$$b'=\begin{pmatrix}\mathbf{b}'_1\\ \mathbf{b}'_2\\ \mathbf{b}'_3\end{pmatrix},\quad b=\begin{pmatrix}\mathbf{b}_1\\ \mathbf{b}_2\\ \mathbf{b}_3\end{pmatrix}$$

and **T** is a 3×3 matrix. Let $\|\mathbf{T}\|$ be the absolute value of the determinant of **T**. We shall call a matrix 'rational' if all its nine elements are rational numbers and 'integral' if all its nine elements are integers. In the Appendix we shall prove the following two theorems.

Theorem 1. Two lattices with bases b and b' have a CSL in common if and only if the matrix $\mathbf{T}$ satisfying $b'=\mathbf{T}b$ is rational.

In the following we assume that $\mathbf{T}$ is rational. If primitive cells of the two lattices have different volumes we choose as number 1 the lattice with the smaller cell volume and have therefore $||\mathbf{T}||\geq 1$.

Theorem 2. Σ_2 is the least positive integer such that $\Sigma_2\mathbf{T}$ and $\Sigma_2||\mathbf{T}||\mathbf{T}^{-1}$ are integral matrices, $\Sigma_1=||\mathbf{T}||\Sigma_2$.

Theorem 2 tells us that Σ_2 can be computed as the least common multiple of the denominators in the 18 elements of $\mathbf{T}$ and of $||\mathbf{T}||\mathbf{T}^{-1}$. If primitive cells of lattices 1 and 2 have equal volumes then Σ $(=\Sigma_1=\Sigma_2)$ is the least common multiple of the denominators in the elements of $\mathbf{T}$ and $\mathbf{T}^{-1}$. Let us compare this result with earlier efforts to determine Σ. Fortes (1972) and Woirgard & de Fouquet (1972) propose methods to determine Σ that apply only if lattices 1 and 2 are related by a rotation and which seem to us more involved than our method. Santoro & Mighell (1973) studied the CLS's generated by arbitrary lattices 1 and 2; they do not give explicit expressions for Σ_1 and Σ_2. If lattices 1 and 2 are primitive cubic and related by a rotation then, choosing conventional bases, $\mathbf{T}^{-1}$ becomes the transpose of $\mathbf{T}$. Theorem 2 then tells us that Σ is the least common multiple of the denominators in the elements of $\mathbf{T}$. A different proof for this special case of Theorem 2 has been given by Grimmer, Bollmann & Warrington (1974).

Examples

To compare the earlier methods with ours, we shall consider some of the examples treated by Fortes (1973) and by Woirgard & de Fouquet (1973). The examples concern the hexagonal lattice with axial ratio $c/a=\sqrt{\frac{8}{3}}$, which corresponds to the h.c.p. structure. We introduce a basis for lattice 1 satisfying

$$\mathbf{b}_1\,.\,\mathbf{b}_1=\mathbf{b}_2\,.\,\mathbf{b}_2=1\,,\quad \mathbf{b}_3\,.\,\mathbf{b}_3=\tfrac{8}{3}$$
$$\mathbf{b}_1\,.\,\mathbf{b}_3=\mathbf{b}_2\,.\,\mathbf{b}_3=0\,,\quad \mathbf{b}_1\,.\,\mathbf{b}_2=-\tfrac{1}{2}\,,$$

and take for lattice 2 the basis b' obtained from b by the rotation we want to consider. For rotations about $\mathbf{b}_1$ we find

$$\mathbf{T}=\begin{pmatrix} 1 & 0 & 0 \\ \dfrac{\cos\omega-1}{2} & \cos\omega & \dfrac{3\sqrt{2}}{8}\sin\omega \\ -\dfrac{2\sqrt{2}}{3}\sin\omega & -\dfrac{4\sqrt{2}}{3}\sin\omega & \cos\omega \end{pmatrix}.$$

$\mathbf{T}^{-1}$ is obtained on replacing ω by $-\omega$. Theorem 2 tells us then that Σ equals the least common multiple of the denominators of

$$\frac{\cos\omega-1}{2}\,,\ \cos\omega\,,\ \frac{3\sqrt{2}}{8}\sin\omega\,,\ \text{ and } \frac{2\sqrt{2}}{3}\sin\omega\,.$$

Taking for tan $(\omega/2)$ the same seven values as Fortes (1973) and Woirgard & de Fouquet (1973), we easily confirm their results. Still another method has been used by Warrington (1975) to determine the rotations that for the hexagonal lattice with $c/a=\sqrt{\frac{8}{3}}$ lead to CSL's with $\Sigma\leq 50$.

The next example will show that $\mathbf{T}$ and $\mathbf{T}^{-1}$ do not always have the same least common multiple of the denominators appearing in the nine matrix elements. If $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ are orthonormal vectors, take $\mathbf{b}_1=9\mathbf{e}_1$, $\mathbf{b}_2=\mathbf{e}_2$, $\mathbf{b}_3=3\mathbf{e}_3$ and $\mathbf{b}_1'=9\mathbf{e}_2$, $\mathbf{b}_2'=\mathbf{e}_3$, $\mathbf{b}_3'=3\mathbf{e}_1$. A 120° rotation about the axis $\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3$ maps lattice 1 onto lattice 2 and b onto b'. The matrix $\mathbf{T}$ describing this rotation is

$$\mathbf{T}=\begin{pmatrix} 0 & 9 & 0 \\ 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 \end{pmatrix} \quad\text{and}\quad \mathbf{T}^{-1}=\begin{pmatrix} 0 & 0 & 3 \\ \frac{1}{9} & 0 & 0 \\ 0 & 3 & 0 \end{pmatrix}.$$

The least common multiples of the denominators are 3 and 9 respectively, $\Sigma=9$.

Determination of the coincidence-site lattice

The explicit determination of a basis for the CSL is particularly easy if we know bases b and b' of lattices 1 and 2 such that $\mathbf{b}_1=\mathbf{b}_1'$. We always know such bases if the two lattices are related by a rotation because then we can choose $\mathbf{b}_1=\mathbf{b}_1'$ parallel to the rotation axis. $\mathbf{T}$ will be of the form

$$\mathbf{T}=\begin{pmatrix} 1 & 0 & 0 \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix}.$$

Let t be the least common multiple of the denominators of t_{21}, t_{22}, and t_{23}. There exists a unique integer n satisfying $0\leq n<t$ such that the numbers $n_i=nt_{2i}+(\Sigma_2/t)t_{3i}$ are integral for $i=1,2,3$. A basis for the CSL is formed by

$$\mathbf{b}_1',\quad t\mathbf{b}_2',\quad \text{and}\quad n\mathbf{b}_2'+(\Sigma_2/t)\mathbf{b}_3'.$$

To find a basis of the CSL in the case $\mathbf{b}_1=\mathbf{b}_1'$ we therefore compute Σ_2 according to Theorem 2 and try out which of the t integers n between 0 and $t-1$ has the property stated above.

This method to determine the CSL explicitly (at least if lattices 1 and 2 are related by a rotation) can be used also to find the DSC lattice, *i.e.* the lattice of the geometrically possible Burgers vectors for dislocations lying in the grain boundary. In fact, the CSL and the DSC lattice are related by a reciprocity relation as has been shown by Grimmer (1974).

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APPENDIX

To prove Theorem 1, assume first that $b'=\mathbf{T}b$, where $\mathbf{T}$ is rational. Let N be the least positive integer such that $N\mathbf{T}$ is integral. $w=Nb'=N\mathbf{T}b$ denotes a triple $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$ of vectors that span a cell of the CSL, which will not be primitive in general. It remains to prove the converse: we assume now that the lattices with bases b and b' have a CSL in common and we let v be a basis for it. It follows that $\mathbf{M}$ and $\mathbf{M}'$ defined by $v=\mathbf{M}b=\mathbf{M}'b'$ are integral matrices. Writing $b'=\mathbf{T}b$ it follows that $\mathbf{T}=\mathbf{M}'^{-1}\mathbf{M}$. $||\mathbf{M}'||$ being a positive integer, and $||\mathbf{M}'||\mathbf{M}'^{-1}$ as well as $\mathbf{M}$ being integral, matrices, we conclude that $\mathbf{T}$ is rational.

To prove Theorem 2, we make use of the following special form of a theorem on the 'elementary divisors' of an integral matrix (see for example: Rédei, 1967; van der Waerden, 1970).

Elementary divisor theorem. Consider two lattices with bases B and B' such that $B'=\mathbf{E}B$, where $\mathbf{E}$ is an integral matrix without a divisor common to all the nine elements. There exist new bases for these lattices, $\hat{B}$ and $\hat{B}'$ respectively, such that the matrix $\hat{\mathbf{E}}$ satisfying $\hat{B}'=\hat{\mathbf{E}}\hat{B}$ is diagonal.

$$\hat{\mathbf{E}}=\begin{pmatrix} e_1 & 0 & 0 \\ 0 & e_2 & 0 \\ 0 & 0 & e_3 \end{pmatrix},$$

where $e_1=1$, e_2=the largest common divisor of the nine elements of $||\mathbf{E}||\mathbf{E}^{-1}$, $e_3=||\mathbf{E}||/e_2$.

Before applying this theorem to our problem, we shall deal with the special case that $\mathbf{T}$ is integral. Then the CSL coincides with lattice 2, $\Sigma_1=||\mathbf{T}||$ and $\Sigma_2=1$. Since $||\mathbf{T}||\geq 1$ prevents $\mathbf{T}^{-1}$ from being integral, when $\mathbf{T}$ is not integral we can now assume that neither $\mathbf{T}$ nor $\mathbf{T}^{-1}$ are integral. Let N and N' be the least positive integers such that $\mathbf{T}_0=N\mathbf{T}$ and $\mathbf{T}_0'=N'\mathbf{T}^{-1}$ respectively are integral matrices. Applying the elementary divisor theorem with $B=b$ (the basis of lattice 1) and $\mathbf{E}=\mathbf{T}_0$, we conclude: there exist new bases $\hat{b}$ and $\hat{b}'$ for lattices 1 and 2 such that $\hat{\mathbf{T}}$, the matrix satisfying $\hat{b}'=\hat{\mathbf{T}}\hat{b}$ has the form

$$\hat{\mathbf{T}}=\begin{pmatrix} t_1 & 0 & 0 \\ 0 & t_2 & 0 \\ 0 & 0 & t_3 \end{pmatrix},$$

where $t_j=\frac{e_j}{N}$ and $e_2=\frac{||\mathbf{T}_0||}{NN'}$,

$$i.e.\ t_1=\frac{1}{N},\ t_2=\frac{N||\mathbf{T}||}{N'},\ t_3=N'.$$

Writing $t_2=p/q$, where p and q are integers without common divisor, we conclude that a basis of the CSL is given by

$$N\hat{\mathbf{b}}_1'=\hat{\mathbf{b}}_1,\quad q\hat{\mathbf{b}}_2'=qN||\mathbf{T}||/N'\hat{\mathbf{b}}_2,\quad \hat{\mathbf{b}}_3'=N'\hat{\mathbf{b}}_3,$$

and that $\Sigma_1=qN||\mathbf{T}||$, $\Sigma_2=qN$. $n=qN$ is the least positive integer such that $n\mathbf{T}$ and $n||\mathbf{T}||\mathbf{T}^{-1}$ are integral matrices. This completes the proof of Theorem 2.

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