approach outlined in this paper. The predicted diffraction effects based on the computer simulation approach do not affect the main conclusion of Pandey *et al.* (1980*a*) that the $2H$ to $6H$ transformation in SiC occurs by the layer displacement mechanism.

References

AHLERS, M. & PLEGRINA, J. L. (1992). *Acta Met. Mater.* **40**, 3213–3220.
CARDELLINI, F. & MAZZONE, G. (1993). *Philos. Mag.* **A67**, 1289.
DEMIN, S. A., NEKRASOV, A. A. & USTINOV, A. I. (1993). *Acta Met. Mater.* **41**, 2091–2095.
FREY, F. & BOYSEN, H. (1981). *Acta Cryst*, **A37**, 819–826.
HITZENBERGER, C., KARNTHALER, H. P. & KORNER, A. (1985). *Acta Met. Mater.* **33**, 1293–1305.
HOLLOWAY, H. (1969). *J. Appl. Phys.* **40**, 4313–4321.
JAGODZINSKI, H. (1971). *Kristallogr.* **16**, 1235–1246.
JEPPS, N. W. & PAGE, T. F. (1980). *J. Microsc.* **119**, 177–188.
KABRA, V. K. & PANDEY, D. (1988). *Phys. Rev. Lett.* **61**, 1493–1496.
KABRA, V. K., PANDEY, D. & LELE, S. (1986). *J. Mater. Sci.* **21**, 1654–1666.
KABRA, V. K., PANDEY, D. & LELE, S. (1988). *J. Appl. Cryst.* **21**, 935–942.
KRISHNA, P. & MARSHALL, R. C. (1971*a*). *J. Cryst. Growth*, **9**, 319–325.
KRISHNA, P. & MARSHALL, R. C. (1971*b*). *J. Cryst. Growth*, **11**, 147–150.
MINAGAWA, T. (1978). *J. Appl. Cryst.* **11**, 243–247.
MUTO, S., VAN TENDELOO, G. & AMELINCKX, S. (1993). *Philos. Mag.* **B67**, 443–463.
NIKOLIN, B. I., BABKEVICH, A. YU., IZDKOVSKAYA, T. V. & PETROVA, S. N. (1993). *Acta Met. Mater.* **41**, 513–515.
OGBUJI, L. U., MITCHELL, T. E. & HEUER, A. H. (1981). *J. Am. Ceram. Soc.* **64**, 91–99.
PANDEY, D. (1976). PhD thesis, Banaras Hindu Univ., India.
PANDEY, D. (1984). *Acta Cryst.* **B40**, 567–569.
PANDEY, D., KABRA, V. K. & LELE, S. (1986). *Bull. Miner.* **109**, 49–67.
PANDEY, D. & KRISHNA, P. (1976). *Acta Cryst.* **A32**, 488–492.
PANDEY, D. & KRISHNA, P. (1982). *Current Topics in Materials Science*, Vol. 9, edited by E. KALDIS, pp. 415–491. Amsterdam: North-Holland.
PANDEY, D. & KRISHNA, P. (1983). *Prog. Cryst. Growth Charact.* **7**, 213–252.
PANDEY, D. & LELE, S. (1986). *Acta Metall.* **34**, 405–413, 415–424.
PANDEY, D., LELE, S. & KRISHNA, P. (1980*a*). *Proc. R. Soc. London Ser. A*, **369**, 435–449.
PANDEY, D., LELE, S. & KRISHNA, P. (1980*b*). *Proc. R. Soc. London Ser. A*. **369**, 451–461.
PANDEY, D., LELE, S. & KRISHNA, P. (1980*c*). *Proc. R. Soc. London Ser. A*, **369**, 463–477.
SEBASTIAN, M. T., PANDEY, D. & KRISHNA, P. (1982). *Phys. Status Solidi A*, **71**, 633–640.
WILSON, A. J. C. (1942). *Proc. R. Soc. London Ser. A*, **180**, 277–285.

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Arithmetic Properties of Module Directions in Quasicrystals, Coincidence Modules and Coincidence Quasilattices

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Abstract

Two new concepts are introduced that are useful for the classification of grain boundaries of quasicrystals: the coincidence module and the coincidence quasilattice. Related to these concepts is the distribution of lengths in different directions of a quasicrystalline module, which, for quasicrystals whose geometry is based on quadratic irrational numbers, is determined by an arithmetic form of the type $sx^2 - y^2$, where s is a square-free integer.

1. Introduction

Rotation of two identical lattices with respect to each other leads, for some special values of the rotation angle, to coincidences of the vertices. In the case of normal crystals, these coincident vertices form the coincidence-site lattice (CSL) (Friedel, 1964; Warrington & Buffalini, 1971; Grimmer, Bollmann & Warrington, 1974). The CSL is important in crystallography because it allows a nontrivial classification of grain boundaries and because small-unit-cell CSL grain boundaries seem to be energetically favoured (see, for instance, Sutton & Balluffi, 1987).

It has been shown (Warrington, 1992, 1993*a*,*b*) that coincidences of the vertices appear also in quasicrystalline tilings. We give here some geometrical tools needed for the study of coincidences in quasicrystals. We first introduce in a unifying perspective the projection schemes for quasicrystals based on quadratic irrationalities, then discuss the concepts of the coincidence module

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and quasirational rotations, which are generalizations of the concepts of coincidence-site lattice and coincidence rotation (Grimmer & Warrington, 1985). We show that the existence of coincidences in quasicrystals is connected to the commensurability of different module directions. The commensurability classes of module directions add to the classification scheme given by Radulescu [1993; hereinafter referred to as (I)]. Some results from (I) are discussed again here, in a more general framework. We also present within the cut-and-projection method (see, for instance, Katz & Duneau, 1986) the concept of the coincidence quasilattice, which is the set of coincidences in a quasiperiodic tiling.

2. Bravais module of quasicrystals

Diffraction from quasicrystals gives Bragg peaks that have as support a finite rank module $L^{\|*}$, the Fourier module. With certain conditions (discussed later), $L^{\|*}$ is the projection onto a d-dimensional physical space $E^{\|}$ of an n-dimensional hyperlattice L^* (reciprocal hyperlattice) from E_n, the n-dimensional Euclidean space $n > d$. The dual of L^* is the Bravais hyperlattice L and the projection of L onto $E^{\|}$ is the Bravais module $L^{\|}$. If L is a primitive hypercubic lattice,† $L^{\|}$ and $L^{\|*}$ differ only by a scale factor.

The Bravais module is a generalization of the Bravais lattice of normal crystals. Although quasicrystals are not periodic structures, atomic rows and planes of quasicrystals are parallel to module directions and planes of the Bravais module [Kupke, Peschke, Carstanjen & Trebin, 1991; (I)]. In particular, the vertices of quasicrystalline tilings obtained by cut and projection (Katz & Duneau, 1986) are discrete subsets of the Bravais module.

Let $\{\mathbf{e}_i^{\|}\}_{i=1,n}$ be a set of generators of $L^{\|}$, $L^{\|} = \{\sum_{i=1}^{n} z_i \mathbf{e}_i^{\|}, z_i \in \mathbb{Z}\}$ and let Γ be its metric matrix, $\Gamma_{i,j} = (\mathbf{e}_i^{\|}, \mathbf{e}_j^{\|})^{\|}$, where $(*, *)^{\|}$ stands for the dot product in $E^{\|}$. Let us further suppose that Γ satisfies the following three conditions that are valid for all the experimentally interesting symmetries (octagonal, decagonal, dodecagonal, icosahedral):

($C1$) Hadwiger's condition $\Gamma^2 = \Gamma$ (see Coxeter, 1963).

($C2$) Irrationality condition $\Gamma \mathbf{u} = \mathbf{u}$, $\mathbf{u} \in L \Rightarrow \mathbf{u} = 0$.

($C3$) Quadratic irrationality condition $\Gamma = \mathbf{A} + \mathbf{B}s^{1/2}$, where $\mathbf{A}$ and $\mathbf{B}$ are symmetrical commuting rational matrices and s is a square-free number (*i.e.* a number that has no squares among its divisors).

($C1$) implies that Γ is the projector onto $E^{\|}$, and the set of generators $\{\mathbf{e}_i^{\|}\}_{i=1,n}$ is the projection onto $E^{\|}$ of the canonical basis $\{\mathbf{e}_i\}_{i=1,n}$ of E_n; $L^{\|} = \Gamma L$, where $L = \{\sum_{i=1}^{n} z_i \mathbf{e}_i\}$ is the n-dimensional hypercubic lattice. ($C2$) implies that $E^{\|}$ has an irrational orientation with respect to L. From ($C1$) and ($C3$), it follows that $\Gamma^{\perp} = \mathbf{A} - \mathbf{B}s^{1/2}$ is an orthogonal projector onto the d-dimensional hyperplane $E^{\perp}$ (the perpendicular space). The fact that $\mathbf{A}$ and $\mathbf{B}$ commute means that $E^{\|}$ and $E^{\perp}$ are orthogonal ($\Gamma \Gamma^{\perp} = 0$).

† The cases with centrings are easy generalizations of the case presented here.

We can show (Appendix 1) that the matrices $\mathbf{A}$ and $\mathbf{B}$ must have a particular form, namely:

($P1$)

$$\mathbf{A} = \mathbf{S}^2/2s, \quad \mathbf{B} = \mathbf{S}/2s,$$

where $\mathbf{S}$ is a symmetrical traceless rational matrix, satisfying the equations

$$\mathbf{S}^3 = s\mathbf{S}, \quad \mathrm{Tr}(\mathbf{S}^2) = 2sd \tag{2.1}$$

$$\Gamma = (1/2s)(\mathbf{S}^2 + s^{1/2}\mathbf{S}), \quad \Gamma^{\perp} = (1/2s)(\mathbf{S}^2 - s^{1/2}\mathbf{S}). \tag{2.2}$$

$$\mathbf{S}\Gamma = \Gamma\mathbf{S} = s^{1/2}\Gamma, \quad \mathbf{S}\Gamma^{\perp} = \Gamma^{\perp}\mathbf{S} = -s^{1/2}\Gamma^{\perp}. \tag{2.3}$$

We can also show (Appendix 1) the existence of a rotation matrix $\mathbf{U}$, such that:

($P2$)

$$\Gamma^{\perp} = \mathbf{U}\Gamma\mathbf{U}^{-1}$$

$$\mathbf{US} + \mathbf{SU} = 0. \tag{2.4}$$

Actually, $\mathbf{S}$ and $\mathbf{U}$ are integer matrices in all cases of interest, a fact that we adopt as a fourth condition:

($C4$) $\mathbf{S}$ is an integer matrix, $\mathbf{U} \in SL(n, \mathbb{Z})$.

Some consequences of ($P1$) are contained in ($P3$) and ($P4$):

($P3$) $E^{\|} \oplus E^{\perp}$ is a $2d$-dimensional hyperplane of E_n and $L_o = E^{\|} \oplus E^{\perp} \cap L$ is a $2d$-dimensional lattice hyperplane of L. The rank of $L^{\|}$ is $2d$ ($L^{\|}$ is therefore a dense set in $E^{\|}$). The projection $L_o^{\|} = \Gamma L_o$ is a submodule of $L^{\|}$, which also has rank $2d$ and therefore a finite index in $L^{\|}$. $L_o^{\|}$ is used in order to define 'colours' of different vectors of $L^{\|}$ as follows: All vectors belonging to $L_o^{\|}$ are declared 'black'. Then, we associate a colour with any coset in $L^{\|}/L_o^{\|}$. Let E^{Δ} be the $(n-2d)$-dimensional orthogonal complement of $E^{\|} \oplus E^{\perp}$ in E_n. E^{Δ} is parallel to a lattice hyperplane of L, $L_{\Delta}^{e} = E^{\Delta} \cap L$. We define the 'colour' lattice $L_{\Delta}^{p} = \Gamma^{\Delta} L$.

$$\Gamma^{\Delta} = 1 - (\mathbf{S}^2/s) \tag{2.5}$$

is the projector onto E^{Δ}.

We show (Appendix 1) that $L^{\|}/L_o^{\|} \simeq L_{\Delta}^{p}/L_{\Delta}^{e}$ and that the number of colours (index of $L_o^{\|}$ in $L^{\|}$) is equal to the square of the volume of the primitive unit cell of L_{Δ}^{e}. If $n = 2d$, there is no $E^{\Delta}(\Gamma^{\Delta} = 0)$, the number of colours is 1 and $\mathbf{S}$ satisfies a simpler relationship: $\mathbf{S}^2 = s\mathbf{1}$ ($\mathbf{1}$ is the identity), which is a particular case of (2.1).

($P4$) $L_o^{\|}$ and $L_o^{\perp} = \Gamma^{\perp} L_o$ are both modules of rank $2d$ and we can define a natural isomorphism between them, as follows (Katz & Duneau 1986): $\mathbf{J} = \Gamma^{\perp}(\Gamma)^{-1}$. According to (2.2),

$$\mathbf{Ju} = \bar{\mathbf{u}}, \tag{2.6}$$

where $\bar{\mathbf{u}}$ is the algebraic conjugate of $\mathbf{u}$.

$\mathbf{J}$ is nowhere continuous and cannot be extended to a linear transformation. $\mathbf{J}$ is of course different from $\mathbf{U}$, which is linear and, like $\mathbf{J}$, transforms $L_o^{\|}$ into $L_o^{\perp}$.

We mention that ($s = 5$, $n = 6$, $d = 3$) in the icosahedral case, ($s = 2$, $n = 4$, $d = 2$) in the octagonal case, ($s = 5$, $n = 5$, $d = 2$) in the decagonal case, ($s = 3$, $n = 6$, $d = 2$) in the dodecagonal case* (see Appendix 1).

3. Quasirational rotations

A rotation $\mathbf{R}^{\|}$ in the physical space produces coincidences in the Bravais module if an only if $\mathbf{R}^{\|}\mathbf{e}_i^{\|} = \sum q_{ij}\mathbf{e}_j^{\|}$, $q_{ij} \in \mathbb{Q}$ (Warrington, 1992, 1993*a*,*b*). We call this type of rotation a *quasirational rotation* and the set of coincidences the *coincidence module* $C^{\|} = L^{\|} \cap \mathbf{R}^{\|}L^{\|}$. $C^{\|}$ is a submodule of $L^{\|}$ and we can define the *coincidence ratio* $\Sigma^{\|}$ as the index of $C^{\|}$ in $L^{\|}$.

An equivalent definition of quasirational rotations can be given if we introduce the concept of the rational space of a module. We call *rational space* $L_Q^{\|}$ of a module $L^{\|}$ the set of all combinations with rational coefficients of vectors in the module: $L_Q^{\|} = \sum_{i=1}^{n} q_i\mathbf{e}_i^{\|}$, $q_i \in \mathbb{Q}$. A quasirational rotation with respect to a module $L^{\|}$ is that rotation which leaves the rational space globally invariant:

$$\mathbf{R}^{\|}L_Q^{\|} = L_Q^{\|}. \tag{3.1}$$

We can also define a rational space L_Q of the hyperlattice L, in the way we did for $L^{\|}$. Let us call the generalized rotations $\mathbf{R}[\mathbf{R} \in \mathrm{O}(n)]$ that leave L_Q invariant *rational generalized rotations* and define the *coincidence hyperlattice* as $C = L \cap \mathbf{R}L$. The *coincidence ratio* Σ in the hyperspace is defined as the index of C in L.

For a given quasirational rotation $\mathbf{R}^{\|}$, there is always a rational generalized rotation $\mathbf{R}$, such that any coincidence in $L^{\|}$ produced by $\mathbf{R}^{\|}$ is the projection of a coincidence in L produced by $\mathbf{R}$ and reciprocally any coincidence in L produced by $\mathbf{R}$ projects onto a coincidence in $L^{\|}$ produced by $\mathbf{R}^{\|}$. $\mathbf{R}$ must necessarily commute with the matrix $\mathbf{S}$. In this case, we have $\Gamma C = C^{\|}$, $\Sigma = \Sigma^{\|}$ and

$$\mathbf{R} = \mathbf{R}^{\|} \oplus \mathbf{R}^{\perp} \oplus \mathbf{R}^{\Delta}, \tag{3.2}$$

where $\mathbf{R}^{\perp}$ is a quasirational rotation in $E^{\perp}$ and $\mathbf{R}^{\Delta}$ is a symmetry of L_{Δ}^{p}, the 'colour' lattice.

Even if by definition $\det(\mathbf{R}^{\|}) = 1$, $\mathbf{R}^{\Delta}$ can be improper and $\det(\mathbf{R}) = \det(\mathbf{R}^{\Delta}) = \pm 1$ if $n > 2d$, both types of rational generalized rotations being possible.

If $d = 3$ and the rotation axis of $\mathbf{R}^{\|}$ is $\mathbf{r}^{\|}$, then the rotation axis of $\mathbf{R}^{\perp}$ is $\mathbf{r}^{\perp} = J\mathbf{r}^{\|}$. The rotation angles $\varphi^{\|}$, $\varphi^{\perp}$ are generally different (formulae that are valid for $d = 2, 3$):

$$\cos(\varphi^{\|}) = (1/4s)[\mathrm{Tr}(\mathbf{RS}^2) + s^{1/2}\mathrm{Tr}(\mathbf{RS})] + 1 - (d/2),$$
$$\cos(\varphi^{\perp}) = (1/4s)[\mathrm{Tr}(\mathbf{RS}^2) - s^{1/2}\mathrm{Tr}(\mathbf{RS})] + 1 - (d/2). \tag{3.3}$$

The proof of all these properties can be found in Appendix 2.

Let us call *quasirational generalized rotations* those rational generalized rotations R that have the form (3.2).

4. Module directions

4.1 *Hyperlattice transversal planes and module directions*

For a better understanding of quasirational rotations, let us discuss the concept of module direction. We call module direction the set of all vectors in a module that are collinear with a given vector. In modules satisfying the conditions ($C1$)–($C3$), all module directions are rank-two modules. It was shown by Katz & Duneau (1986) and discussed again by us in (I) that [($C1$)–($C3$) being true] module directions are projections onto $E^{\|}$ of one (when $n = 2d$) two-dimensional lattice plane $P \subset E^{\|} \oplus E^{\perp}$ or several two-dimensional lattice planes $P_i = P + r_i$, $r_i \in L^p$ (one for each colour), which are transversal with respect to $E^{\|}$, $E^{\perp}$ [they are parallel to $E^{\|} \oplus E^{\perp}$ and are 'on the edge' when looking from $E^{\|}$ and from $E^{\perp}$, *i.e.* $P \cap E^{\|} = \Gamma(P^{\|})$ and $P \cap E^{\perp} = \Gamma^{\perp}(P^{\perp})$]. We called these planes [see (I)] hyperlattice transversal planes (HTP).

4.2 *Arithmetic classes of module directions*

As the lengths in a module direction form a dense set, there is no smallest length as in normal crystals. Nevertheless, in a module direction, we have periodic series of lengths $n\mathbf{r}^{\|}$, $n \in \mathbb{Z}$, generated by the projections of primitive vectors $\mathbf{r} \in L$. Any two lengths belonging to different series are incommensurate. Some series are generated by $\mathbf{r}^{\|}$ vectors that are black, and contain only black vectors. Other series are 'coloured' (they are generated by a 'coloured' $\mathbf{r}^{\|}$ vector). Because $\forall\, \mathbf{r} \in L$, $\mathbf{S}^2\mathbf{r} \in L_o$ and $\Gamma\mathbf{S}^2\mathbf{r} = s\Gamma\mathbf{r}$, in a coloured series, we have a black point after each s coloured points. We can pass from one series generated by $\mathbf{a}^{\|}$ to any other series generated by $\mathbf{b}^{\|}$ ($\mathbf{a}^{\|}$ and $\mathbf{b}^{\|}$ are collinear) by multiplying the lengths of the first series by $qs^{1/2} + p, p, q \in \mathbb{Z}$ (we eventually obtain a commensurate subseries generated by $k\mathbf{b}^{\|}$, $k \in \mathbb{Z}$). Using (2.3), we show that this similarity corresponds in the hyperspace to the application of $q\mathbf{S} + p\mathbf{1}$ to the vector $\mathbf{r} \in L$.

Let us denote by $P(p,q;\mathbf{r})$ and $P(\mathbf{r})$ the lengths of the projections onto $E^{\|}$ of $(q\mathbf{S} + p\mathbf{1})\mathbf{r}$ and of $\mathbf{r}$, respectively. Using (2.2) and (2.3) [see also (I)], we show that

$$P(p, q; \mathbf{r}) = (qs^{1/2} + p)P(\mathbf{r})$$
$$P(\mathbf{r}) = \{[x(\mathbf{r})s + y(\mathbf{r})]/2s^{1/2}\}, \tag{4.1}$$

* Although the minimal dimension of a lattice L that gives by projection a dodecagonal or a decagonal module is 4 (Niizeki, 1989), the orthogonality condition (symmetry of the matrix $\mathbf{S}$) demands minimal dimensions 6 and 5, respectively, of the Bravais hyperlattice L.

where

$$x(\mathbf{r}) = (1/s)(\mathbf{r}, \mathbf{S}^2\mathbf{r}) = (1/s)\sum S_{ik}S_{kj}x_i x_j \qquad (4.2)$$

$$y(\mathbf{r}) = (\mathbf{r}, \mathbf{S}\mathbf{r}) = \sum S_{ij}x_i x_j, \qquad (4.3)$$

if $\mathbf{r} = \sum x_i \mathbf{e}_i$, $x_i \in \mathbb{Z}$.

For those $\mathbf{r}$ that project onto black vectors, $\mathbf{r} \in L_o$ and, from (2.5),

$$x(\mathbf{r}) = (\mathbf{r}, \mathbf{r}) = \sum x_i^2. \qquad (4.4)$$

In (I) we have also discussed the values of the angles $O(p, q; \mathbf{r})$ formed by $(q\mathbf{S} + p\mathbf{1})\mathbf{r}$ and by $\mathbf{r}$ with the physical space, for $\mathbf{r} \in L_o$. These angles are important for the geometry of the rational approximants of quasicrystals and satisfy:*

$$\tan\theta(p, q; \mathbf{r}) = [(p - qs^{1/2})/(p + qs^{1/2})]\tan\theta(\mathbf{r})$$
$$\tan\theta(\mathbf{r}) = \{[x(\mathbf{r})s^{1/2} - y(\mathbf{r})]/[x(\mathbf{r})s^{1/2} + y(\mathbf{r})]\}^{1/2}. \qquad (4.5)$$

We introduced [see (I)] the concept of compatibility of module directions, which is an equivalence relation between module directions. We call two module directions compatible if there exists a black vector $\mathbf{r}_1^{\parallel}$ on the first module direction and a black vector $\mathbf{r}_2^{\parallel}$ on the second module direction such that

$$\tan\theta(\mathbf{r}_1) = \tan\theta(\mathbf{r}_2). \qquad (4.6)$$

We also showed in (I) that there is a simple arithmetic compatibility criterion. Let $f(\mathbf{r}) = sx^2(\mathbf{r}) - y(\mathbf{r})^2$ be a biquadratic integer-valued form defined on L_o. We have a unique decomposition of the form

$$f(\mathbf{r}) = n_1(\mathbf{r})n_2^2(\mathbf{r})n_3^4(\mathbf{r}), \qquad (4.7)$$

where $n_1(\mathbf{r})$, $n_2(\mathbf{r})$ are square-free integers. $n_1(\mathbf{r})$ (which we call the compatibility index) is the same for all vectors $\mathbf{r} \in L_o$ projecting onto the same module direction and the compatibility condition is written $n_1(\mathbf{r}_1) = n_1(\mathbf{r}_2)$.

Let us here rename the compatibility the *angle* compatibility in order to distinguish it clearly from another equivalence relation, which we introduce subsequently. We call two module directions commensurate if there exist two commensurate lengths, one in the first direction, the other in the second direction: $P(\mathbf{r}_1)/P(\mathbf{r}_2) = p/q$, $p, q \in \mathbb{Z}$.

As any vector on a module direction is commensurate with a black vector ($\mathbf{S}^2\mathbf{r} \in L_o \forall\ \mathbf{r} \in L$), we can consider, without losing generality, that $\mathbf{r}_1$ and $\mathbf{r}_2$ are black.

Using (4.1) and (4.5), we show that the ratios of lengths of black vectors in two module directions are square-rooted rationals if and only if (4.6) is satisfied and therefore the module directions are angle compatible. In this case, $P(\mathbf{r}_1)/P(\mathbf{r}_2) = [n_2(\mathbf{r}_1)/n_2(\mathbf{r}_2)]^{1/2}[n_3(\mathbf{r}_1)/n_3(\mathbf{r}_2)]$. Therefore, in order to have commensurability, we must have angle compatibility and $n_2(\mathbf{r}_1) = n_2(\mathbf{r}_2)$. In this case not only is the series of lengths containing $\mathbf{r}_1^{\parallel}$ commensurate with the series of lengths containing $\mathbf{r}_2^{\parallel}$, but any series in one module direction is commensurate with a series in the other module direction (all these series are produced by similarities $qs^{1/2} + p$ from a given one). In order to obtain a commensurability criterion that is independent of the series chosen on the module direction $\mathbf{r}^{\parallel}$, we define a new index $n_2^r(\mathbf{r})$, which we call the commensurability index and which is obtained from $n_2(\mathbf{r})$ by elimination of all square-free factors of the form $p^2 - sq^2$. The commensurability criterion is $n_2^r(\mathbf{r}_1) = n_2^r(\mathbf{r}_2)$, where $n_2^r(\mathbf{r})$ does not change for different vectors $\mathbf{r} \in L_o$ projecting onto the same module direction.*

To conclude, let us note that commensurability implies angle compatibility, but this is not true conversely. For instance, in an icosahedral Bravais module,† twofold, threefold, fivefold and $[\tau 10]$ axes ($[\tau 10]$ is an axis making an orthogonal base with a fivefold and a twofold axis) have indices (n_1, n_2^r) equal to (1,1), (1,3), (5,1) and (5,1), respectively. In consequence, fivefold and $[\tau 10]$ axes are angle compatible and commensurate, but threefold and twofold axes are only angle compatible.

* A rational approximant is a structure that is formed with the same stuctural units as the quasicrystal, but in a periodic arrangement.

* The proof uses results from Mordell (1969) and is given by Radulescu (1994).

† There are in fact three types of icosahedral modules: P, F and C types, which come respectively from primitive (P), face-centred (F) and body-centred (C) hypercubic hyperlattices (Rokshar, Mermin & Wright 1987). As all these types of modules have the same rational space, the classes of module directions are the same.

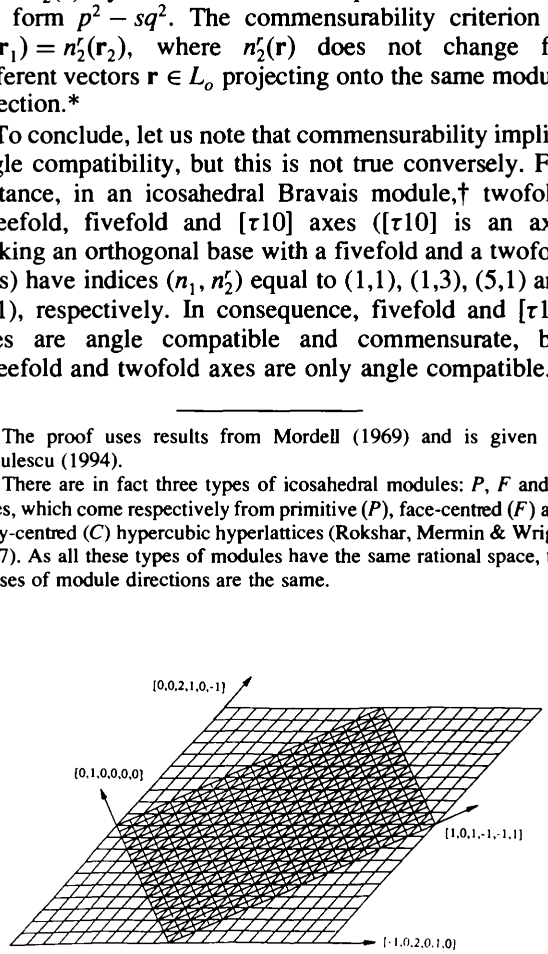


Fig. 1. For an icosahedral module, the rotation

$$\mathbf{R} = \tfrac{1}{2}\begin{bmatrix} 1 & 1 & -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & -1 & 1 & 1 \\ 1 & 0 & 0 & -1 & -1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & -1 & 1 & 0 & 1 & 0 \\ 0 & -1 & -1 & 1 & 0 & 1 \end{bmatrix} \quad (\varphi^{\parallel} = 90°,\ \varphi^{\perp} = 90°)$$

conserves the HTP containing $[0, 0, 0, -1, 0, 1]$ (the rotation axis in the physical space is the projection of this HTP) and transforms the HTP containing $[0, 1, 0, 0, 0, 0]$ (projecting onto a fivefold axis in physical space) into the HTP containing $[-1, 0, 2, 0, 1, 0]$ (projecting onto a $[\tau 10]$ axis in physical space).

The connection between quasirational rotations and classes of module directions is such that a quasirational rotation necessarily transforms module directions into module directions belonging to the same commensurability class, in order to produce coincidences on all module directions. The form (3.2) of a quasirational rotation means also that quasirational rotations permute colours but transform black vectors into black vectors.

The quasirational generalized rotations carry HTPs into commensurate HTPs (we call two HTPs commensurate if they correspond to commensurate module directions) and produce two-dimensional coincidence lattices in each of these HTPs (Fig. 1). In particular, the HTP corresponding to the rotation axis $d^{\|}$ is kept fixed.

5. Coincidence quasilattice

A quasiperiodic tiling can be obtained by cut and projection (Katz & Duneau, 1986) from the hyperlattice. The vertices of the quasiperiodic tiling form a discrete subset of the Bravais module.

The same quasirational rotations that produce coincidences in the Bravais module produce coincidences in the quasiperiodic tiling also. We call the set of coincidences in the tiling the coincidence quasilattice (Fig. 2).

$$C_q = T \cap \mathbf{R}^{\|}T, \qquad (5.1)$$

where T is the quasiperiodic tiling, obtained by cut and projection.

$$T = \Gamma[L \cap (D + E^{\|})]; \qquad (5.2)$$

$D + E^{\|}$ is called the strip and D is the acceptance domain (usually the interior of one or several polytopes in $E^{\perp} \oplus E^{\Delta}$).

Using (5.1) and (5.2), we show that C_q is obtained by cut and projection from the coincidence hyperlattice with the acceptance domain $D^* = D \cap \mathbf{R}^{\perp}D : C_q = \Gamma[C \cap (D^* + E^{\|})]$.

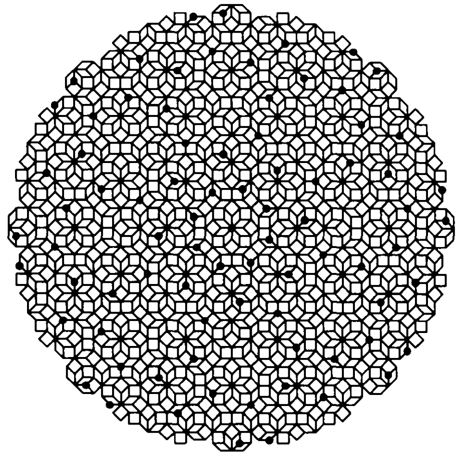
We notice that the ratio Σ_a (actual coincidence ratio) of the density of points in T to the density of points in C_q is greater than Σ by a factor that is the ratio of the volumes of D and D^*; if D is close to a sphere and the rotation $\mathbf{R}^{\perp}$ is around an axis that passes through the centre $\mathbf{r}_d^{\perp}$ of this sphere, then this factor is close to one (Fig. 3).

Σ and Σ_a depend both on the position $\mathbf{r}_c^{\|}$ of the rotation axis of $\mathbf{R}^{\|}$ and on $\mathbf{r}_d^{\perp}$. $\mathbf{r}_c^{\|}$ and $\mathbf{r}_d^{\perp}$ are relative to the origins of $\mathbf{L}^{\|}$ and $\mathbf{L}_o^{\perp}$, respectively. First of all, there are coincidences if and only if $\mathbf{r}_c^{\|}$ satisfies

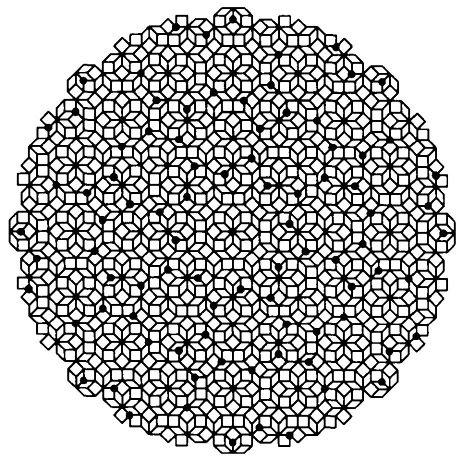
$$\mathbf{R}^{\|}(\mathbf{r}_c^{\|} + \mathbf{r}_1^{\|}) = \mathbf{r}_c^{\|} + \mathbf{r}_2^{\|}, \dagger \qquad (5.3)$$

where $\mathbf{r}_1^{\|}, \mathbf{r}_2^{\|} \in L^{\|}$. The proof of this condition uses the property that a rotation around an axis that passes through $\mathbf{r}_c^{\|}$ is equal to the rotation about the origin, followed by a translation $\mathbf{r}_c^{\|} - \mathbf{R}^{\|}\mathbf{r}_c^{\|}$. We use the same property to show that for all rotation axes satisfying (5.3) the value of Σ is the same. All the translation vectors $\mathbf{r}_c^{\|} \in L^{\|}$ satisfy (5.3), but there are some vectors from $L_Q^{\|} - L^{\|}$ that also satisfy (5.3). For instance, turning the tiling in Fig. 2 around a vertex (which belongs to $L^{\|}$) or around the centre of a square tile (which does not belong to $L^{\|}$, but belongs to $L_Q^{\|}$) produces the

† This condition means that $\mathbf{r}_c^{\|}$ and $\mathbf{R}^{\|}\mathbf{r}_c^{\|}$ belong to the same coset of $L_Q^{\|}/L^{\|}$.



(a)



(b)

Fig. 2. Nonequivalent coincidence quasilattices $\Sigma = 17$ in an octagonal tiling (CSL vertices designated with dots). The rotation matrices are equivalent by a symmetry of the hyperlattice, which is not a symmetry of the Bravais module (matrix $\mathbf{U}_o$ in Appendix 1).

$$(a)\,\mathbf{R} = \tfrac{1}{17}\begin{bmatrix} 6 & 12 & -10 & -3 \\ 3 & 6 & 12 & -10 \\ 10 & 3 & 6 & 12 \\ 12 & 10 & 3 & 6 \end{bmatrix} (\varphi^{\|} = 12.35^\circ, \varphi^{\perp} = 105.72^\circ);$$

$$(b)\,\mathbf{R} = \tfrac{1}{17}\begin{bmatrix} 6 & -3 & 10 & 12 \\ -12 & 6 & -3 & 10 \\ -10 & -12 & 6 & -3 \\ 3 & -10 & -12 & 6 \end{bmatrix} \varphi^{\|} = 105.72^\circ, \varphi^{\perp} = 12.35^\circ);$$

same density of coincidences in the module (same value of Σ).

For a finite given value of Σ [so for $\mathbf{r}_c^{\parallel}$ satisfying (5.3)], Σ_a depends on the difference between $\mathbf{r}_c^{\perp}$, the position of the rotation axis in $E^{\perp}$ ($\mathbf{r}_c^{\perp} = \mathbf{J}\mathbf{r}_c^{\parallel}$), and $\mathbf{r}_d^{\perp}$. Σ_a takes a minimum value if $\mathbf{r}_d^{\perp} = \mathbf{r}_c^{\perp}$, and is infinite (no coincidences) if D and $\mathbf{R}^{\perp}D$ are disjoint (see Fig. 3).

6. Equivalence of quasirational rotations

The main object studied in the crystallography of grain boundaries is the bicrystal (Bollmann, 1970), which is the superposition of the two rotated Bravais lattices of the grains. In our case, the 'biquasicrystal' is $B = T \cup \mathbf{R}^{\parallel}T$. This representation is not unique because of the symmetry of the grains: $B = \mathbf{G}_1^{-1}(T \cup \mathbf{G}_1\mathbf{R}^{\parallel}\mathbf{G}_2^{-1}T)$, where $\mathbf{G}_1$, $\mathbf{G}_2 \in G_Q^{\parallel}$, $G_Q^{\parallel}$ being the symmetry group of the quasicrystal. In analogy with Warrington & Buffalini (1971), we call two quasirational rotations equivalent if $\mathbf{R}_2^{\parallel} = \mathbf{G}_1\mathbf{R}_1^{\parallel}\mathbf{G}_2^{-1}$, $\mathbf{G}_1, \mathbf{G}_2 \in G_Q^{\parallel}$.

Equivalent quasirational rotations generate equivalent coincidence quasilattices and coincidence modules, which have of course the same values of Σ. The equivalence of generalized rotations is defined in the same way:

$$\mathbf{R}_2 = \mathbf{G}_1\mathbf{R}_1\mathbf{G}_2^{-1}, \quad \mathbf{G}_1, \mathbf{G}_2 \in G_Q, \tag{6.1}$$

where G_Q is an embedding of $G_Q^{\parallel}$ in the holohedry $H(L)$ of L.

The symmetries G_Q and the generalized inflations* $p\mathbf{S}^2 + q\mathbf{S} + r\mathbf{1}$, $p, q, r \in Z$ are elements of $H(L)$ that commute with $\mathbf{S}$ (see Janssen, 1990):

$$\mathbf{GS} - \mathbf{SG} = 0. \tag{6.2}$$

* A generalized inflation is a transformation from L to L, which acts as a similarity in $E^{\parallel}$ and $E^{\perp}$. If $s = 4k + 1$, then p and q can also be half-integers. The generalized inflations contain the 'true' inflations (Janssen, 1990), which are invertible and, therefore, unimodular.

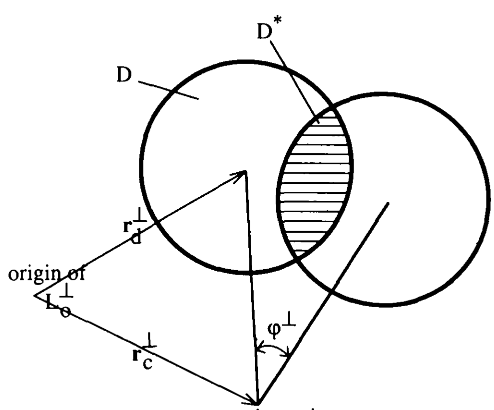


Fig. 3. Dependence of Σ_a on the positions $\mathbf{r}_c^{\perp}$, $\mathbf{r}_d^{\perp}$ of the rotation axis and of the acceptance domain D in the perpendicular space; Σ_a is proportional to the inverse of the hatched volume D^*.

We can, in certain cases, obtain coincidence quasilattices that are nonequivalent, but that have the same value of Σ if $\mathbf{G}_1$, $\mathbf{G}_2$ in (6.1) are replaced by the transformations $\mathbf{T}_1$, $\mathbf{T}_2$ that belong to $H(L)$ but that anticommute with $\mathbf{S}$ (both $\mathbf{R}_1$ and $\mathbf{R}_2$ must commute with $\mathbf{S}$):

$$\mathbf{ST} + \mathbf{TS} = 0. \tag{6.3}$$

A transformation that satisfies (6.3) is of the form $\mathbf{T} = \mathbf{T}_o\mathbf{U}$, where $\mathbf{T}_o$ is a generic transformation that satisfies (6.2), and $\mathbf{U}$ is a particular transformation that satisfies (6.3) and therefore interchanges the physical and the perpendicular space [see ($P2$) and Appendix 1]. $\mathbf{U}R\mathbf{U}^{-1}$ have permuted values of $\varphi^{\perp}, \varphi^{\parallel}$, but the same value of Σ. If $\varphi^{\perp} = \varphi^{\parallel}$, $\mathbf{URU}^{-1}$ is still equivalent to $\mathbf{R}$. It is only the case $\varphi^{\perp} \neq \varphi^{\parallel}$ that can lead to a degeneracy of Σ (nonequivalent coincidence quasilattices; see Fig. 2).

7. Concluding remarks

For quasicrystals, quasirational rotations generalize coincidence rotations from the crystallography of normal crystals. The coincidence module and the coincidence quasilattice generalize the concept of coincidence site lattice. We have developed in this paper the geometrical framework for the study of coincidence modules and coincidence quasilattices.

The quasirational rotations for an important class of quasicrystals (those whose geometry is governed by quadratic irrational numbers) are related to a form $sx^2 - y^2$. Module directions can be classified according to their arithmetic properties in angle-compatibility classes and commensurability classes; the class indices are given by the form $sx^2 - y^2$.

We showed that there is some degeneracy of the values of the coincidence ratios, which is due to symmetries of the hyperlattice, which are not symmetries of the quasicrystal.

An extensive presentation of coincidence modules and quasilattices, including coincidence ratios in the case of the icosahedral symmetry, will be addressed in a forthcoming paper (Warrington, Radulescu & Lück, in preparation).

The analysis here is interesting in itself, but may be useful for the classification of grain boundaries in quasicrystals. The coincidence quasilattice (and any cut through it) is quasiperiodic, which means that grain boundaries in quasicrystals must be quasiperiodic. The experimental study of grain boundaries in quasicrystals is at its very beginning, the only special disorientations which have been reported are $\Sigma = 5$ (Singh & Ranganathan 1993; Dai & Urban, 1993), $\Sigma = 11$ (Warrington, 1988, 1993b) in icosahedral quasicrystals.

After submission of this paper we learned of a paper by Pleasants, Baake & Roth (1994) treating the CSL problem for planar modules with n-fold symmetry by using prime factorization in cyclotomic fields. The approach that we have presented is complementary.

APPENDIX 1

The matrices $\mathbf{A}$ and $\mathbf{B}$ must satisfy

$$(\mathbf{A}+\mathbf{B}s^{1/2})^2 = \mathbf{A}+\mathbf{B}s^{1/2}, \qquad (A1.1)$$
$$i.e.\ \mathbf{A}^2 + s\mathbf{B}^2 = \mathbf{A}, \quad 2\mathbf{AB} = \mathbf{B}.$$

As $\mathbf{A}$ and $\mathbf{B}$ are symmetrical and commute, they can be simultaneously diagonalized in some algebraic extension of $\mathbf{Q}$. If $\mathbf{Au} = \lambda\mathbf{u}, \mathbf{Bu} = \mu\mathbf{u}$, then $\lambda^2 + s\mu^2 = \lambda$, $2\lambda\mu = \mu$, a system that has the following solutions:

$$\begin{aligned} \mu &= 0, & \lambda &= 1 \\ \mu &= 0, & \lambda &= 0 \\ \mu &= \pm 1/2s^{1/2}, & \lambda &= \tfrac{1}{2}. \end{aligned} \qquad (A1.2)$$

The first solution $(A1.2)$ is forbidden by condition $(C2)$, the other two imply that $\mathbf{A} = 2s\mathbf{B}^2$, $\mathbf{B}^3 = (1/4s)\mathbf{B}$. If $\mathbf{S} = 2s\mathbf{B}$, then $\mathbf{A} = (1/2s)\mathbf{S}^2$, $\mathbf{B} = (1/2s)\mathbf{S}$, $\mathbf{S}^3 = s\mathbf{S}$ and, because $\Gamma = (1/2s)(\mathbf{S}^2 + s^{1/2}\mathbf{S})$ is a projector on a hyperplane of dimension d, $\mathrm{Tr}(\mathbf{S}^2) = 2sd$, $\mathrm{Tr}(\mathbf{S}) = 0$.

In order to define the matrix $\mathbf{U}$, we proceed as following: Let $\mathbf{U}|_{\mathrm{Ker}\mathbf{S}} = 1$. Let P_i, $i = 1, d$, be d mutually orthogonal HTPs ($P_i \subset E^{\parallel} \oplus E^{\perp}$), corresponding to d mutually orthogonal module directions $\mathbf{u}_i$. $\mathbf{S}$ has the form $\left[\begin{smallmatrix} s^{1/2} & 0 \\ 0 & -s^{1/2}\end{smallmatrix}\right]$ in the basis $(\mathbf{u}_i, \bar{\mathbf{u}}_i = \mathbf{J}\mathbf{u}_i)$. Then, $\mathbf{U}$ must be of the form $\left[\begin{smallmatrix} 0 & a \\ b & 0\end{smallmatrix}\right]$ in order to satisfy $\mathbf{US} + \mathbf{SU} = 0$. Therefore, the restriction of $\mathbf{U}$ to P_i must be either a $\pi/2$ rotation or a reflection in a plane whose normal lies in P_i and makes an angle $\pi/4$ with $\mathbf{u}_i$.

A rotation of $\pi/2$ in an HTP is a rational rotation if and only if the index $n_1 = 1$. In this case, for any vector $\mathbf{r} \in P_i \cap L_o$, $\mathbf{r}' = [n_1(\mathbf{r})^{1/2} n_2(\mathbf{r}) n_3^2(\mathbf{r})]^{-1}[(\mathbf{r}, \mathbf{Sr})\mathbf{r} - (\mathbf{r}, \mathbf{r})\mathbf{Sr}]$ is rational, orthogonal to $\mathbf{r}$ and $\|\mathbf{r}\| = \|\mathbf{r}'\|$ [see $(P1)$, (4.4) and (4.7)]. A reflection in a plane making an angle $\pi/4$ with $\mathbf{u}_i$ is rational if and only if the vector $\mathbf{r}$ making an angle $\pi/4$ with $\mathbf{u}_i$ is rational. But in this case, $y(\mathbf{r}) = 0$ and $n_1(\mathbf{r}) = s$ [see (4.5), (4.7)]. Actually, in all interesting cases, there are d mutually orthogonal directions of indices $n_1 \in \{1, s\}$ and, more than that, $\mathbf{U}$ is an integer matrix. For instance, in the icosahedral case, a twofold, a fivefold and a $[\tau 10]$ axis have indices 1, 5, 5, respectively (§4.2) and $\mathbf{U}$ is composed of a $\pi/2$ rotation in the HTP of the twofold axis and two reflections.

Finally, we give some theorems about colours, which are cosets in $L^{\parallel}/L_o^{\parallel}$. First,

$$L^{\parallel}/L_o^{\parallel} \simeq L_{\Delta}^{p}/L_{\Delta}^{e}. \qquad (A1.3)$$

To show $(A1.3)$, we use the first isomorphism theorem (Hungerford, 1984) and $L \xrightarrow{\Gamma^{\Delta}} L_{\Delta}^{p}$, $L \xrightarrow{\Gamma} L^{\parallel}$, $L_o \xrightarrow{\Gamma} L_o^{\parallel}$, in order to show that $L/L_o \simeq L_{\Delta}^{p}$, $L/L_{\Delta}^{e} \simeq L^{\parallel}$, $L_o \simeq L_o^{\parallel}$, and then the third isomorphism theorem (Hungerford, 1984).

Let $\{\mathbf{a}_i\}_{i=1,n-2d}$ be a primitive basis of L_{Δ}^{e}.

A vector $\mathbf{p}$ in L_{Δ}^{p} is the projection of a vector $\mathbf{r} \in L$, $\mathbf{p} = \Gamma^{\Delta}\mathbf{r}$, therefore has the form $\mathbf{p} = \sum \mathbf{r}_i\mathbf{a}_i$, where the coordinates r_i must satisfy $(\mathbf{r} - \sum r_i\mathbf{a}_i, \mathbf{a}_j) = 0$, $i.e. \sum r_i(\mathbf{a}_i, \mathbf{a}_j) = (\mathbf{r}, \mathbf{a}_j)$. As $\{\mathbf{a}_i\}_{i=1,n-2d}$ is primitive, $x_j = (\mathbf{r}, \mathbf{a}_j)$ can take any integer values. $L_{\Delta}^{e} = \{\sum x_i\mathbf{a}_i | x_i \in \mathbb{Z}\}$, therefore the number of colours is $\#(L_{\Delta}^{p}/L_{\Delta}^{e}) = \det(\mathbf{a}_i, \mathbf{a}_j) = \Omega^2$, Ω being the volume of the primitive cell of L_{Δ}^{e} (# is for cardinal).

The matrices $\mathbf{S}$ and $\mathbf{U}$ and the basis $\{\mathbf{a}_i\}_{i=1,n-2d}$ of L_{Δ}^{e} for icosahedral, octagonal, decagonal and dodecagonal quasicrystals are

$$\mathbf{S}_i = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & -1 & -1 & 1 \\ 1 & 1 & 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 & 1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 1 \\ 1 & 1 & -1 & -1 & 1 & 0 \end{bmatrix},$$

$$\mathbf{U}_i = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{S}_o = \begin{bmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{U}_o = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$

$$\mathbf{S}_{de} = \begin{bmatrix} 0 & 1 & -1 & -1 & 1 \\ 1 & 0 & 1 & -1 & -1 \\ -1 & 1 & 0 & 1 & -1 \\ -1 & -1 & 1 & 0 & 1 \\ 1 & -1 & -1 & 1 & 0 \end{bmatrix},$$

$$\mathbf{U}_{de} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{a}_1^{de} = [1, 1, 1, 1, 1],$$

$$\mathbf{S}_{do} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ -1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{U}_{do} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{a}_1^{do} = [1, 0, -1, 0, 1, 0], \quad \mathbf{a}_2^{do} = [0, 1, 0, -1, 0, 1].$$

APPENDIX 2

Let us show the existence of a matrix $\mathbf{R}$ satisfying the following conditions:

$$(\mathbf{R}\mathbf{r}_1 = \mathbf{r}_2,\ \mathbf{r}_1, \mathbf{r}_2 \in L) \Rightarrow (\mathbf{R}^{\|}\Gamma\mathbf{r}_1 = \Gamma\mathbf{r}_2) \qquad (A2.1)$$

$$(\mathbf{R}^{\|}\mathbf{r}_1^{\|} = \mathbf{r}_2^{\|},\ \mathbf{r}_1^{\|}, \mathbf{r}_2^{\|} \in L^{\|}) \Rightarrow$$
$$(\exists \mathbf{r}_1, \mathbf{r}_2 \in L, \text{ such that } \mathbf{R}\mathbf{r}_1 = \mathbf{r}_2, \mathbf{r}_1^{\|} = \Gamma\mathbf{r}_1, \mathbf{r}_2^{\|} = \Gamma\mathbf{r}_2). \qquad (A2.2)$$

Using (A2.1) and (A2.2), we prove the following theorem:

Theorem 1. $\mathbf{R}$ exists and is of the form $\mathbf{R} = \mathbf{R}^{\|} \oplus \mathbf{R}^{\perp} \oplus \mathbf{R}^{\Delta}$, with $\mathbf{R}^{\|}, \mathbf{R}^{\perp}$ acting in $E^{\|}, E^{\perp}$ and $\mathbf{R}^{\Delta}$ is a symmetry of L_{Δ}^{p}; the angles of $\mathbf{R}^{\|}, \mathbf{R}^{\perp}$ satisfy (3.3).

The proof follows from three lemmas:

Lemma 1. If $\mathbf{r}_1, \mathbf{r}_2 \in L_o$, then $\|\Gamma\mathbf{r}_1\| = (1/k)\ \|\Gamma\mathbf{r}_2\| \Rightarrow (\|\mathbf{r}_1\| = (1/k)\ \|\mathbf{r}_2\|,\ \|\Gamma^{\perp}\mathbf{r}_1\| = (1/k)\ \|\Gamma^{\perp}\mathbf{r}_2\|)$, where $k \in \mathbb{Z}$.

The proof of this lemma follows from (P1) and (4.4).

Lemma 2. $\mathbf{R}L_o = L_o$.

As discussed in §4, for any vector in $L^{\|}$ there is a black vector that is commensurate with it, being s times longer. Therefore, $\mathbf{R}^{\|}$ produces a rank-$2d$ coincidence module in $L_o^{\|}: \exists \mathbf{p}_i^{\|}, \mathbf{q}_i^{\|} \in L_o^{\|}, i = 1, 2d$ such that $\mathbf{R}^{\|}\mathbf{p}_i^{\|} = \mathbf{q}_i^{\|}$. We define $\mathbf{R}$ in order to satisfy (A2.2):

$$\begin{aligned} \mathbf{R}(\mathbf{p}_i + \delta_i^1) &= \mathbf{q}_i + \delta_i^2 \\ \delta_i^1, \delta_i^2 &\in L_{\Delta}^{e}, \mathbf{p}_i, \mathbf{q}_i \in L_o. \end{aligned} \qquad (A2.3)$$

Let us show that we must have

$$\delta_i^2 - \mathbf{R}\delta_i^1 \in L_{\Delta}^{e}. \qquad (A2.4)$$

If this is not true then (A2.3) and (A2.1) imply that $\mathbf{R}^{\|}\mathbf{p}_i^{\|} = \bar{\mathbf{q}}_i^{\|}$, with $\bar{\mathbf{q}}_i^{\|} \neq \mathbf{q}_i^{\|}$. As $\|\mathbf{p}_i^{\|}\| = \|\mathbf{q}_i^{\|}\|$, according to lemma 1, $\|\mathbf{p}_i\| = \|\mathbf{q}_i\|$ and, from (A2.3), (A2.4), $\delta_i^2 - \mathbf{R}\delta_i^1 = 0$. This and ($A$2.3) entail that $\mathbf{R}L_o = L_o$.

Lemma 3. $\mathbf{R}E^{\|} = E^{\|}, \mathbf{R}E^{\perp} = E^{\perp}$.

Consider an arbitrary module direction in $L_o^{\|}$ and a series of vectors in L_o, $\mathbf{r}_n \to \mathbf{r}^{\|} \in L_o^{\|}$. Then, $\mathbf{R}\mathbf{r}_n = (1/k)\mathbf{p}_n$, where $\mathbf{p}_n \in L_o, k \in \mathbb{Z}$. By continuity, $(1/k)\mathbf{p}_n \to \mathbf{R}\mathbf{r}^{\|}$. According to ($A$2.1), $\mathbf{R}^{\|}(\Gamma\mathbf{r}_n) = (1/k)(\Gamma\mathbf{p}_n)$, so that $\|\Gamma\mathbf{r}_n\| = (1/k)\|\Gamma\mathbf{p}_n\|$. Also, $\|\mathbf{r}_n\| = (1/k)\|\mathbf{p}_n\|$, then by Lemma 1, $\|\Gamma^{\perp}\mathbf{r}_n\| = (1/k)\|\Gamma^{\perp}\mathbf{p}_n\|$. As $\|\Gamma^{\perp}\mathbf{r}_n\| \to 0, \|\Gamma^{\perp}\mathbf{p}_n\| \to 0$ and $\mathbf{R}\mathbf{r}^{\|} \in E^{\|}$. This shows that $\mathbf{R}E^{\|} = E^{\|}$. As $\mathbf{R}$ is orthogonal, $\mathbf{R}E^{\perp} = E^{\perp}$ also.

Therefore, $\mathbf{R} = \mathbf{R}^{\|} \oplus \mathbf{R}^{\perp} \oplus \mathbf{R}^{\Delta}$, where $\mathbf{R}^{\Delta}$ is chosen such that it performs the same permutation of colours in L_{Δ}^{p} as $\mathbf{R}^{\|}$ does in $L^{\|}$.

Finally, (3.3) comes from $\mathrm{Tr}(\mathbf{R}\Gamma) = 2\cos(\varphi^{\|}) + d - 2$, and $\mathrm{Tr}(\mathbf{R}\Gamma^{\perp}) = 2\cos(\varphi^{\perp}) + d - 2$, where $d = 2, 3$ is the dimension of the physical space.

Theorem 2. $\mathbf{R}$ satisfies $\Gamma C = C^{\|}$, $\Sigma = \Sigma^{\|}$.

Proof: The first property follows directly from (A2.1) and (A2.2). For the second property, we use the first isomorphism theorem (Hungerford, 1984), $L \xrightarrow{\Gamma} L^{\|}$ and $C \xrightarrow{\Gamma} C^{\|}$ in order to show that $L/L_{\Delta}^{i} \simeq L^{\|}$, $C/L_{\Delta}^{i} \simeq C^{\|}$, and the third isomorphism theorem (Hungerford, 1984) in order to show $L/C \simeq L^{\|}/C^{\|}$, and therefore $\#(L/C) = \#(L^{\|}/C^{\|})$.

Notice that it may happen that $\mathbf{R}^{\|}\mathbf{p}_i^{\|} = \mathbf{q}_i^{\|}$, with $\mathbf{p}_i^{\|}, \mathbf{q}_i^{\|}$ of different colours so that $\mathbf{R}^{\Delta}$ is not necessarily the identity. In this case, the rotation $\mathbf{R} = \mathbf{R}^{\|} \oplus \mathbf{R}^{\perp} \oplus \mathbf{1}^{\Delta}$ ($\mathbf{1}^{\Delta}$ is the identity in E^{Δ}) is also quasirational, but $\Sigma(R)$ is a multiple of $\Sigma^{\|}$ (bicoloured coincidences are skipped).

References

Bollman, W. (1970). *Crystal Defects and Crystalline Interfaces*, p. 143. Berlin: Springer-Verlag.

Coxeter, H. S. M. (1963). *Regular Polytopes*, 2nd ed., p. 250. New York: Macmillan.

Dai, M. X. & Urban, K. (1993). *Philos. Mag. Lett.* **67**, 67–71.

Friedel, G. (1964). *Leçons de Cristallographie*. Paris: Blanchard. (Reprint of 1926 edition.)

Grimmer, H., Bollmann, W. & Warrington, D. H. (1974). *Acta Cryst.* **A30**, 197–207.

Grimmer, H. & Warrington, D. H. (1985). *J. Phys. Paris Colloq.* C4, pp. 231–236.

Hungerford, T. W. (1984). *Algebra*, p. 44. Berlin: Springer-Verlag.

Janssen, T. (1990). In *Quasicrystals, Springer Series in Solid-State Sciences*, Vol. 93, edited by T. Fujiwara & T. Ogawa. Berlin: Springer-Verlag.

Katz, A. & Duneau, M. (1986). *J. Phys. Fr.* **47**, 181–186.

Kupke, T., Peschke, U., Carstanjen, H.-D. & Trebin, H.-R. (1991). *Phys. Rev. B*, **43**, 13758–13761.

Mordell, L. J. (1969). *Diophantine Equations*. New York/London: Academic Press.

NIIZEKI, K. (1989). *J. Phys. A*, **22**, 193–204.
PLEASANTS, P. A. B., BAAKE, M. & ROTH, J. (1994). Tübingen preprint TPT-QC-94-05-1. Univ. Tübingen, Germany.
RADULESCU, O. (1993). *J. Phys. I Fr.* **3**, 2099–2113.
RADULESCU, O. (1994). Thèse, Univ. de Paris Sud, France.
ROKSHAR, D. S., MERMIN, N. D. & WRIGHT, D. C. (1987). *Phys. Rev. B*, **35**, 5487.
SINGH, A. & RANGANATHAN, S. (1993). *J. Non-Cryst. Solids*, **153 & 154**, 86–91.
SUTTON, A. P. & BALLUFFI, R. W. (1987). *Acta Metall.* **35**, 2177–2201.
WARRINGTON, D. H. (1988). *Quasicrystalline Materials*, edited by C. JANOT & J. M. DUBOIS, p. 243. Singapore: World Scientific.
WARRINGTON, D. H. (1992). Colloque Quasicristaux, Meudon, France.
WARRINGTON, D. H. (1993*a*). Colloque Quasicristaux, Grenoble, France.
WARRINGTON, D. H. (1993*b*). Colloque Quasicristaux, Thessaloniki. *Mater. Sci. Forum*, **126–128**, 57–60.
WARRINGTON, D. H. & BUFFALINI, P. (1971). *Scr. Metall.* **5**, 771–776.

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Models for Termination of Crystal Boundaries in the Theory of Transmission Electron Diffraction and Comparison with Experimental Data

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Abstract

Calculations of electron diffraction intensities in transmission electron microscopy commonly assume a model representing surfaces and interfaces in crystals as flat boundaries (flat-boundary model, FBM). It is shown that the independent-atom model (IAM) representing the crystal potential as a superposition of spherical atomic potentials leads to improved boundary conditions. Intensities calculated from the two models at large deviation from the Bragg peak in weak reflections (*e.g.* 200 in InGaAs) differ significantly. Results from both types of calculation are compared with an experimental diffraction pattern recorded using energy-filtered large-angle convergent-beam electron diffraction from an $In_{0.53}Ga_{0.47}/InP$ bicrystal. It is shown that calculations using the IAM give a better agreement with experiment.

1. Introduction

Calculations of electron diffraction intensities from thin crystals in transmission electron microscopy (TEM) usually assume a sharp cut-off of the crystal potential at surfaces and sharp transitions of the potential at interfaces inside the sample. This leads to a convenient set of boundary conditions that can be used in dynamical theory (see Peng & Whelan, 1990*a*, for a recent review). The effects of contamination and the detailed three-dimensional atomic structure of surfaces and interfaces are generally ignored owing to their small contribution to the total volume of the crystal. Earlier attempts at understanding the effect of boundary conditions in multislice calculations have been made for forbidden reflections (Stobbs, Boothroyd & Stobbs, 1989; Gipson, Lanzerotti & Elser, 1989). Here, we report a different representation of the crystal potential which pays more attention to the spatial variation of the potential at the atomic level at interfaces and surfaces. This leads to a significantly improved agreement between calculated and observed intensities in cases where the reflection under consideration is weak, such as the 200 reflection from InGaAs. Contamination is still assumed to play a minor role and is ignored in the calculations.

2. The crystal potential at surfaces and interfaces

In an infinite perfect crystal, the potential can be represented by a Fourier series (Bethe, 1928). Discontinuities at surfaces and interfaces perturb the potential inside the bulk. However, it is usually assumed that these perturbations are confined to a small volume and that the potential in the bulk is unchanged. Thus, the situation can

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