Acta Cryst. (1997). A53, 772–780

Grain Boundaries as Projections from Higher-Dimensional Lattices

J. L. Aragón, D. Romeu, L. Beltrán and A. Gómez*

Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México, Distrito Federal, México. E-mail: alfredo@fenix.ifisicacu.unam.mx

(Received 6 February 1997; accepted 15 May 1997)

Abstract

The problem of finding the points of best fit between pairs of lattices is formulated in higher dimensions and solved using a modified version of the cut and projection method. This best-fit set constitutes a generalization of the concept of coincidence and is relevant to the theory of grain boundaries. It establishes an interesting link between the theory of quasicrystals and grain boundaries.

1. Introduction

Owing to its technological importance, the problem of determining the atomic structure of grain boundaries has been the subject of a considerable amount of work in the last few decades. A number of geometrical models have been proposed with varying degrees of success. All models assume that 'special' boundaries, *i.e.* grain boundaries with special properties, arise when there is a high degree of 'good fit' between the lattices of the parent crystals; for instance, the coincidence site lattice (CSL) (Ranganathan, 1966) considers points common to both lattices (the intersection lattice) as points of good fit and assumes that special boundaries arise when the density of coincidence sites is high. A generalization of the CSL has produced the more successful structural units model (Bishop & Chalmers, 1968), which accounts for the observed relative displacement of the parent crystals that destroys coincidence sites, although it still considers that special boundaries are those with small periods as predicted by the CSL. Another generalization of the CSL is the *O*-lattice theory (Bollmann, 1970), which considers that *O*-points (points with the property of having the same internal coordinates in both lattices) correspond to positions of good fit between the two lattices. In exact coincidence orientations, the *O*-lattice contains the CSL but, in contrast with the latter, it varies continuously over the whole angular range. A related concept is that of the displacement shift complete (DSC) lattice (Bollmann, 1970), which is defined as the sum of the two lattices; Burgers vectors of grain-boundary dislocations are assumed to belong to the DSC lattice. Unfortunately, none of the models proposed so far has been successful in predicting the structure of arbitrary grain boundaries (special or not) and thus the elaboration of a general grain-boundary theory has not been possible.

With the aim of solving this problem, a new generalization of the CSL model, called the generalized coincidence sites network (GCSN) has been introduced (Romeu, Beltrán, Aragón & Gómez, 1997; Gómez, Beltrán, Aragón & Romeu, 1997). The new model provides the atomic structure of arbitrary grain boundaries, including defects such as grain-boundary dislocations and vacancies, and has been successful in describing important experimental observations related to dislocation content and the speciality criterion (Romeu, Beltrán, Aragón & Gómez, 1997; Gómez, Beltrán, Aragón & Romeu, 1997).

In the GCSN model, two points are considered to be good-fit points if they both lie in the intersection of their respective Voronoi (or Wigner–Seitz) cells. Since this condition is obviously met by coincidence points, a GCSN contains the CSL. We stress the term network here since, in contrast with the CSL, GCSN structures need not be periodic. The main difference between GCSN and CSL models, or any other model for that matter, is that it not only provides the positions of special (*e.g.* coincidence) points but it also produces its decoration, thus giving a complete description of the boundary. An interesting point of the new model is that its formalism is similar to that used to produce quasicrystals in the multigrid approach (de Bruijn, 1981; Kramer & Neri, 1984; Levine & Steinhardt, 1986). This establishes a clear link between grain boundaries and quasicrystals that has motivated this work and could provide a new insight into both fields.

This relationship between quasicrystal and grain boundaries had been noticed some years ago. A. P. Sutton (1988) observed that the simplest irrational tilt boundaries may be described as a quasiperiodic sequence of appropriate fundamental structural units. This result was supported by the suggestion (Rivier & Lawrence, 1988) that a quasicrystalline grain boundary has the minimal Gibbs free energy under specific boundary conditions. Finally, it was found useful to consider a six-dimensional lattice to study the symmetries of general grain boundaries in three dimensions (Gratias & Thalal, 1988).

In this work, we show, through the particular case of two rotated square lattices, that the set of GCSN points between a pair of lattices in two or three dimensions can be obtained by projecting points from a higher-dimensional lattice using a modified version of the so-called cut and projection method (Duneau & Katz, 1985). Some tilings associated with the pair of square lattices are obtained by projection and their relation to twist grain boundaries is pointed out. This shows that it is possible to use the powerful tools already developed in the field of quasicrystals, such as the multigrid (de Bruijn, 1981; Kramer & Neri, 1984; Levine & Steinhardt, 1986) and the cut and projection method (Duneau & Katz, 1985) to study the structure of grain boundaries.

The paper is organized as follows. In §2, the theory behind the problem of finding the points of good fit between a pair of arbitrary three-dimensional lattices is presented, showing the relationship between regions of good fit (as defined by the GCSN model), CSL and grain boundaries. In §3, the higher-dimensional approach to the problem is presented and detailed for the case of two rotated square lattices. In §4, we propose a method to find the projection matrix when dealing with arbitrary basis vectors, which implies non-cubic higher-dimensional lattices. The relationship between rational approximants of a quasiperiodic structure and the CSL is developed in §5. Some examples of GCSN's associated with the pair of square lattice are given in §6 and, finally, §7 is devoted to discussion and conclusions.

2. The basic theory

In order to state notation and definitions, in this section we briefly review the theory involved in the problem of finding the points of best fit between a given pair of lattices. A complete and more detailed account of the theory is given elsewhere (Gómez, Beltrán, Aragón & Romeu, 1997). In the present work, attention is restricted to pairs of simple cubic lattices related by means of a rotation where, as will be shown in §3, the connection with higher-dimensional lattices is clearer.

Let L_1 and L_2 be two point lattices with common origin in $\mathbf{R}^3$ having basis vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ and $\{\mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6\}$, respectively. The generic lattice vectors $\mathbf{l}_1 \in L_1$ and $\mathbf{l}_2 \in L_2$ may then be written as

$$\mathbf{l}_1 = \xi_1\mathbf{a}_1 + \xi_2\mathbf{a}_2 + \xi_3\mathbf{a}_3,$$
$$\mathbf{l}_2 = \zeta_1\mathbf{a}_4 + \zeta_2\mathbf{a}_5 + \zeta_3\mathbf{a}_6,$$

where ξ_i and ζ_i are integers.

Let us now consider the following problem: for a lattice L in $\mathbf{R}^3$ and an arbitrary point $\mathbf{x} \in \mathbf{R}^3$, find a lattice point $\mathbf{l}$ that minimizes the distance from $\mathbf{x}$ to $\mathbf{l}$. In other words, find the lattice point $\mathbf{l}$ closest to $\mathbf{x}$. This problem has several practical applications and has been extensively treated (Conway & Sloane, 1988) for important lattices in three or more dimensions. The general solution is directly related to the Voronoi tessellation of the lattice L, that is, $\mathbf{l} \in L$ is the closest lattice point to $\mathbf{x}$ if $\mathbf{x}$ is inside the Voronoi polyhedron around $\mathbf{l}$. For the case of the simple cubic lattices we are dealing with, the solution can be expressed in a compact form: given $\mathbf{x} \in \mathbf{R}^3$, the lattice point in L_1 closest to it is

$$N_1(\mathbf{x}) = \sum_{i=1}^{3} \mathrm{round}(\mathbf{x} \cdot \mathbf{a}_i^*)\mathbf{a}_i, \tag{1}$$

where round(x) is the closest integer to x, with round$(n + \frac{1}{2}) = n$ for integer n and $\{\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*\}$ is the basis reciprocal to $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$. Similarly, the lattice point in L_2 closest to $\mathbf{x}$ is given by

$$N_2(\mathbf{x}) = \sum_{i=4}^{6} \mathrm{round}(\mathbf{x} \cdot \mathbf{a}_i^*)\mathbf{a}_i, \tag{2}$$

where $\{\mathbf{a}_4^*, \mathbf{a}_5^*, \mathbf{a}_6^*\}$ is the basis reciprocal to $\{\mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_5\}$. Notice that the terms round$(\mathbf{x} \cdot \mathbf{a}_i^*)$ are basically the external coordinates of $\mathbf{x}$ in the terminology of Bollmann (1970).

Equations (1) and (2) partition the space in cells. A given point $\mathbf{x} \in \mathbf{R}^3$ belongs to the cell centered around $\mathbf{l}_1 \in L_1$ if $N_1(\mathbf{x}) = \mathbf{l}_1$ with a similar condition holding for L_2. The cell around $\mathbf{l}_1 \in L_1$ will be denoted by $\Lambda_1(\mathbf{l}_1)$ and that around $\mathbf{l}_2$ (with respect to L_2) by $\Lambda_2(\mathbf{l}_2)$. Formally,

$$\Lambda_1(\mathbf{l}_1) = \{\mathbf{x} \in \mathbf{R}^3 | N_1(\mathbf{x}) = \mathbf{l}_1\}$$
$$\Lambda_2(\mathbf{l}_2) = \{\mathbf{x} \in \mathbf{R}^3 | N_2(\mathbf{x}) = \mathbf{l}_2\}.$$

2.1. *Points of good fit between the lattices L_1 and L_2*

In the following, we are interested in finding points of good fit (in a sense specified below) between L_1 and L_2. The key concept in the present model is that of *neighbors*. We say that two lattice points $\mathbf{l}_1 \in L_1$ and $\mathbf{l}_2 \in L_2$ are neighbors if and only if

$$N_1(\mathbf{l}_2) = \mathbf{l}_1,$$
$$N_2(\mathbf{l}_1) = \mathbf{l}_2$$

or, alternatively, if

$$\mathbf{l}_1, \mathbf{l}_2 \in \Lambda_1(\mathbf{l}_1) \cap \Lambda_2(\mathbf{l}_2). \tag{3}$$

The model postulates that, if the atoms are centered at the positions of L_1 in one grain and L_2 in the other, atoms at the boundary are at positions of good fit between the two lattices where these positions are in turn given by the set

$$\mathcal{G} = \{(\mathbf{l}_1 + \mathbf{l}_2)/2 | \mathbf{l}_1 \in L_1, \mathbf{l}_2 \in L_2, \quad \mathbf{l}_1, \mathbf{l}_2 \text{ are neighbors}\}, \tag{4}$$

which has been referred to as the generalized coincidence sites network or GCSN.

The idea behind this approach is that the points of good fit between two lattices are always half way between a point in the first lattice and a point in the second lattice provided that they are close to each other in the sense of being neighbors. Also note that, by construction, if there is a coincidence relationship between the two lattices, the set of coincidence sites is a subset of $\mathcal{G}$.

It should be remarked that, for non-cubic lattices, equations (1) and (2) must be formulated in terms of the Voronoi polyhedron around the lattice points $\mathbf{l}_1$ and $\mathbf{l}_2$, respectively, instead of using the round function. In the present case, it is important to notice that the points in $\mathcal{G}$ are of the form

$$[N_1(\mathbf{x})+N_2(\mathbf{x})]/2=\tfrac{1}{2}\left(\sum_{i=1}^{3}\operatorname{round}(\mathbf{x}\cdot\mathbf{a}_i^*)\mathbf{a}_i + \sum_{i=4}^{6}\operatorname{round}(\mathbf{x}\cdot\mathbf{a}_i^*)\mathbf{a}_i\right), \qquad (5)$$

an expression that resembles that used in the grid formulation of quasilattices (Levine & Steinhardt, 1986).

2.2. *Lattice displacements*

In the most general case, the lattices do not have to possess a common origin and one may be displaced with respect to the other. Assume that L_1 has its origin at the origin of the coordinate system, as before, but the origin of L_2 is displaced by vector $\mathbf{t}$ with respect to the origin of the coordinate system. In this case, the formalism still applies, but for instance $N_2(\mathbf{x})$ will be given by $\sum_{i=4}^{6}\operatorname{round}[(\mathbf{x}-\mathbf{t})\cdot\mathbf{a}_i^*]\mathbf{a}_i$. The terms $\mathbf{t}\cdot\mathbf{a}_i^*$ are similar to the phason terms in the jargon of quasicrystals (Levine & Steinhardt, 1986).

2.3. *Comparison with Bollmann's O-lattice theory*

Given the lattices L_1 and L_2, if A is the linear mapping such that $A(\mathbf{a}_i)=\mathbf{a}_{i+3}$ $(i=1,2,3)$, then (Smith & Pond, 1976) $\mathbf{O}$ is an O-point if and only if it satisfies $(I-A^{-1})\mathbf{O}=\mathbf{l}_1$ for some $\mathbf{l}_1\in L_1$ (I represents the identity mapping). The O-points have the property that, if an O-point $\mathbf{O}$ is used as the new origin for the coordinate system, the transformation A still generates L_2 from L_1 around $\mathbf{O}$.

The bases for L_1 and L_2 and the transformation A should be chosen in such a way that, in a neighborhood of the origin, A relates closest points [*i.e.* if $\mathbf{l}_1\in L_1$ then $A(\mathbf{l}_1)$ is the point in L_2 closest to $\mathbf{l}_1$]. If the whole space is partitioned by the Voronoi cells of the O-lattice, then within each cell, given $\mathbf{l}_1\in L_1$, we can find the point in L_2 closest to it, namely $A(\mathbf{l}_1)$. The points $\mathbf{l}_1$ and $A(\mathbf{l}_1)$ would be, in our terminology, neighbors.

Bollmann proposes the use of a linear relaxation model to construct the boundary (Bollmann, 1982). A boundary point is assumed to lie on the line joining $\mathbf{l}_1$ and $A(\mathbf{l}_1)$ but its exact location should be chosen in such a way that for regions on the boundary close to lattice L_1 the boundary atom should lie close to $\mathbf{l}_1$, whereas for regions on the boundary close to lattice L_2 the boundary atom should be close to $A(\mathbf{l}_1)$.

The GCSN coincides with the model by Bollmann if the boundary atom is assumed to be located at $[\mathbf{l}_1+A(\mathbf{l}_1)]/2$. However, in its most general formulation (not the restricted version applicable only to simple cubic lattices presented here), the GCSN has a number of distinct advantages:

(i) There is no need to select bases for the lattices. In this way, there is no ambiguity due to the non-uniqueness of the bases.

(ii) The transformation A is not used at all, here again there is no ambiguity owing to the non-uniqueness of the transformation relating the lattices.

(iii) The GCSN works adequately for any pair of lattices. There are no problems when the lattices are related by rotations (or shears) where the matrix $(I-A^{-1})$ does not have an inverse.

(iv) The GCSN can be used not only for arbitrary pairs of lattices but also for noncrystalline structures such as quasicrystals. In the GCSN, any two Delaunay systems (Galiulin, 1980) can be studied.

3. Projection from higher-dimensional spaces

It has already been mentioned that the equations describing the GCSN model [equation (5)] are closely related to those used in the multigrid method (de Bruijn, 1981; Kramer & Neri, 1984; Levine & Steinhardt, 1986). Thus, the question arises of whether the set of points generated using equations (5) or (4) can also be obtained by projection from higher-dimensional spaces, in exactly the same way as quasilattices can be obtained by the cut and projection method (Duneau & Katz, 1985). Actually, as we shall show below, the problem of finding the points of good fit of a given pair of cubic lattices can be adequately formulated and solved in higher dimensions using the cut and projection method.

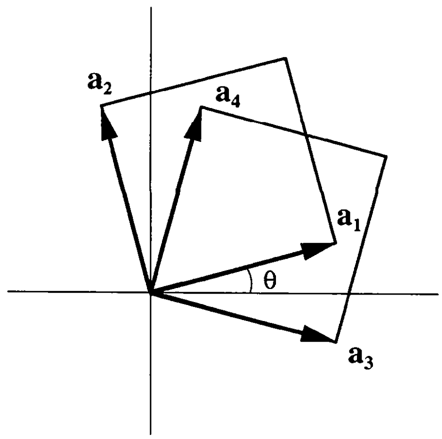


Fig. 1. Basis vectors of the two square lattices considered in this work. The lattice L_1 is generated by $\{\mathbf{a}_1,\mathbf{a}_2\}$ and L_2 by $\{\mathbf{a}_3,\mathbf{a}_4\}$.

To introduce the basic ideas used in this approach, we shall consider the simple case of two square lattices in the plane rotated by a given angle. Let L_1 and L_2 be two lattices generated by $\{\mathbf{a}_1, \mathbf{a}_2\}$ and $\{\mathbf{a}_3, \mathbf{a}_4\}$, respectively, and given by

$$\begin{aligned}\mathbf{a}_1 &= 2^{-1/2}(\cos\theta, \sin\theta),\\ \mathbf{a}_2 &= 2^{-1/2}(-\sin\theta, \cos\theta),\\ \mathbf{a}_3 &= 2^{-1/2}(\cos\theta, -\sin\theta),\\ \mathbf{a}_4 &= 2^{-1/2}(\sin\theta, \cos\theta).\end{aligned} \tag{6}$$

As shown in Fig. 1, these vectors generate two square lattices rotated by 2θ.

The first step towards a higher-dimensional formulation consists in viewing L_1 and L_2 as the intersection points of a two-dimensional grid g defined as the union of four systems g_i of equidistant parallel lines defined as

$$g_i = \{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \cdot \mathbf{a}_i = k_i, \quad k_i = 0, \pm 1, \pm 2, \ldots\}, \qquad i = 1, 2, 3, 4.$$

If $\mathbf{l}_1 \in L_1$, then $\mathbf{l}_1$ is the intersection of lines $\mathbf{y} \cdot \mathbf{a}_i = k_i$, where $i = 1, 2$, and, if $\mathbf{l}_2 \in L_2$, then it is the intersection of lines $\mathbf{y} \cdot \mathbf{a}_i = k_i$, where $i = 3, 4$.

According to the discussion above, equations (1) and (2) partition the space in cells. The grid g^* associated with these cells is the Voronoi tessellation of g, which turns out to be the union of the systems

$$g_i^* = \{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \cdot \mathbf{a}_i = (k_i + 1/2), \quad k_i = 0, \pm 1, \pm 2, \ldots\}, \qquad i = 1, 2, 3, 4.$$

So, for instance, the primitive translation cell of g^*, which corresponds to the primitive cell that equation (1) defines for L_1, is

$$\{\mathbf{y} \in \mathbf{R}^2 | -\tfrac{1}{2} < \mathbf{y} \cdot \mathbf{a}_i \leq \tfrac{1}{2}, \quad i = 1, 2\}.$$

Similarly, for L_2,

$$\{\mathbf{y} \in \mathbf{R}^2 | -\tfrac{1}{2} < \mathbf{y} \cdot \mathbf{a}_i \leq \tfrac{1}{2}, \quad i = 3, 4\}.$$

Now, let G be a four-dimensional grid consisting of four systems of hyperplanes defined as

$$G_i = \{y \in \mathbf{R}^4 | y \cdot e_i = k_i, \quad k_i = 0, \pm 1, \pm 2, \ldots\}, \qquad i = 1, 2, 3, 4,$$

where $\{e_1, e_2, e_3, e_4\}$ is the canonical (orthonormal) basis of $\mathbf{R}^4$. The intersection points of G define a four-dimensional cubic lattice $\mathcal{L}$ with a primitive translational cell given by

$$\{y \in \mathbf{R}^4 | 0 < y \cdot e_i \leq 1, \quad i = 1, 2, 3, 4\}.$$

Let us now consider an orthogonal decomposition of $\mathbf{R}^4$ as $\mathbf{R}^4 = E^{\|} + E^{\perp}$, such that $E^{\|} = \mathbf{R}^2$ is the space of the grid g. The connection between g and G arises when one identifies g with the intersection of $E^{\|}$ with the four-dimensional grid G, that is

$$g = \{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \in G \cap E^{\|}\}. \tag{7}$$

This directly lead us to the grid method originally proposed by de Bruijn (1981) to generate quasiperiodic tilings of the plane and generalized by Kramer & Neri (1984) to three-dimensional grids. In this formalism, a quasiperiodic (or periodic) tessellation of the plane or space is obtained as the dual of the grid g.

3.1. *Neighborhood criterion*

The neighborhood criterion expressed by equation (3) for a pair of lattice points $\mathbf{l}_1 \in L_1$ and $\mathbf{l}_2 \in L_2$ can now be formulated. First note that the Voronoi tessellation of G is

$$G_i^* = \{y \in \mathbf{R}^4 | y \cdot e_i = (k_i + \tfrac{1}{2}), \quad k_i = 0, \pm 1, \pm 2, \ldots\}, \qquad i = 1, 2, 3, 4. \tag{8}$$

Since in this case their intersection points define also a cubic lattice but displaced by $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, g^* is obtained as

$$g^* = \{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \in G^* \cap E^{\|}\}.$$

Now, let $l_1^{\|} \in L_1$ and $l_2^{\|} \in L_2$ be the coordinates of $\mathbf{l}_1$ and $\mathbf{l}_2$ embedded in $\mathbf{R}^4$. According to equation (7), $l_1^{\|}$ and $l_2^{\|}$ can be written as

$$\begin{aligned}l_1^{\|} &= \{y \in \mathbf{R}^4 | y \cdot e_i = k_i, \quad i = 1, 2\} \cap E^{\|},\\ l_2^{\|} &= \{y \in \mathbf{R}^4 | y \cdot e_i = k_i, \quad i = 3, 4\} \cap E^{\|}.\end{aligned}$$

From equation (8), the cells around $l_1^{\|}$ and $l_2^{\|}$ are, respectively,

$$\begin{aligned}\Lambda_1(l_1^{\|}) &= \{y \in \mathbf{R}^4 | (k_i - \tfrac{1}{2}) < y \cdot e_i \leq (k_i + \tfrac{1}{2}),\\ &\qquad i = 1, 2\} \cap E^{\|},\\ \Lambda_2(l_2^{\|}) &= \{y \in \mathbf{R}^4 | (k_i - \tfrac{1}{2}) < y \cdot e_i \leq (k_i + \tfrac{1}{2}),\\ &\qquad i = 3, 4\} \cap E^{\|},\end{aligned}$$

with which $\Lambda_1(l_1^{\|}) \cap \Lambda_2(l_2^{\|})$ becomes

$$\Lambda_1(l_1^{\|}) \cap \Lambda_2(l_2^{\|}) = \{y \in \mathbf{R}^4 | (k_i + \tfrac{1}{2}) < y \cdot e_i \leq (k_i + \tfrac{1}{2}), \quad i = 1, 2, 3, 4\} \cap E^{\|},$$

which is the intersection of $E^{\|}$ with a cell of G^* with index (k_1, k_2, k_3, k_4). If the neighborhood criterion [see equation (3)] is such that $l_1^{\|}, l_2^{\|} \in \Lambda_1(l_1^{\|}) \cap \Lambda_2(l_2^{\|})$, it implies that $l_1^{\|}$ and $l_2^{\|}$ must lie in a cell of G^*. In other words, $\mathbf{l}_1$ and $\mathbf{l}_2$ are neighbors if, embedded in $\mathbf{R}^4$, both lie in a cell of G^*.

It can easily be seen that in our case of hypercubic lattices if $l_1^{\|}$ and $l_2^{\|}$ both lie in a cell of G^* then

$$\operatorname{round}(l_1^{\|} \cdot e_i) = \operatorname{round}(l_2^{\|} \cdot e_i), \quad i = 1, 2, 3, 4. \tag{9}$$

Fig. 2 illustrates a low-dimensional example of the above procedure. Care must be taken in this case since in all the previous formulations the set (6) generates two identical square lattices rotated with respect to each other. This fact (and the eutacticity of the star) allows us to use a four-dimensional cubic hyperlattice, defined as the intersection points of G, in such a way that the plane grid is viewed as the intersection of $E^{\parallel}$ with G. In the case depicted in Fig. 2, we cannot reproduce the situation of two rotated lattices generated by a star of vectors of the same norm. Instead, we have to consider to linear lattices L_1 and L_2 with parameters $a_1 = 1$ and $a_2 = \tau$, respectively. The one-dimensional 'grid' g is in this case the union of the systems $g_i = \{y \in \mathbf{R} | ya_i = k_i, k_i = 0, \pm1, \pm2, \ldots\}$, $i = 1, 2$, which is viewed as the intersection with the two-dimensional rectangular grid G formed by the union of the systems $G_i = \{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \cdot \boldsymbol{\varepsilon}_i = k_i, \quad k_i = 0, \pm1, \pm2, \ldots\}, \quad i = 1, 2$, where $||\boldsymbol{\varepsilon}_1|| = 1/2^{1/2}$ and $||\boldsymbol{\varepsilon}_2|| = \tau/2^{1/2}$. Thus, the space containing L_1 and L_2 is embedded in $\mathbf{R}^2$ in such a way that vertices of $\mathbf{L}_1$ are the intersections of $E^{\parallel}$ with the grid $\{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \cdot \boldsymbol{\varepsilon}_1 = k_i\}$ (vertical lines) and vertices of L_2 are the intersections of $E^{\parallel}$ with the grid $\{\mathbf{y} \in \mathbf{R}^2 | \mathbf{y} \cdot \boldsymbol{\varepsilon}_2 = k_i\}$ (horizontal lines). The Voronoi tessellation of the two-dimensional rectangular lattice is drawn with broken lines and pairs of points fulfilling the neighborhood condition [equation (9)] lie in the shaded Voronoi cells. The projection, onto $E^{\parallel}$, of the centers of these cells gives the GCSN of L_1 and L_2. As will be shown in the next section, the projected points constitute a subset of those obtained by the cut and projection method and the GCSN is therefore, in this example, a subset of the Fibonacci chain.

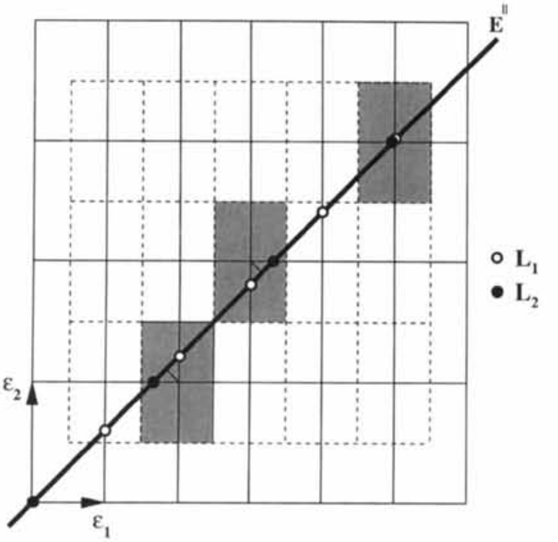


Fig. 2. One-dimensional example of the procedure described in the text to obtain the best-fit lattice of a pair of lattices. In this case, two linear chains L_1 and L_2 with different parameters ($a_1 = 1$ and $a_2 = \tau$) are embedded in $\mathbf{R}^2$. The vertices of L_1 (L_2) are the intersections of $E^{\parallel}$ with the vertical (horizontal) lines of the two-dimensional grid with spacings $1/2^{1/2}$ and $\tau/2^{1/2}$, respectively. The Voronoi tessellation of the two-dimensional lattice is drawn with broken lines and the pairs of points fulfilling the neighborhood condition lie in the shaded Voronoi cells. The projection (onto $E^{\parallel}$) of the centers of these cells gives the best-fit lattice between L_1 and L_2.

3.2. *The cut and projection method*

The connection between the cut and projection and the grid methods becomes clear when one considers the four-dimensional lattice $\mathcal{L}$ and the projections, onto $E^{\parallel}$, of the lowest-coordinate corners of the cubes of $\mathcal{L}$ that have non-zero intersection with $E^{\parallel}$. These are the vertices of the tiling associated with the grid g, *i.e.* the quasiperiodic tiling. The set of vertices of $\mathcal{L}$ to be projected lies inside a strip parallel to $E^{\parallel}$. This is the same strip that the cut and projection method considers (Gähler & Rhyner, 1986).

In this context, the neighborhood criterion (9) can be rewritten as follows. Since $\sum_{i=1}^{4} \mathrm{round}(l_1^{\parallel} \cdot e_i)e_i$ and $\sum_{i=1}^{4} \mathrm{round}(l_2^{\parallel} \cdot e_i)e_i$ are vertices of $\mathcal{L}$, say x_1 and x_2, the condition (9) requires that $x_1 = x_2 = x$. This imposes a restriction on the magnitude of the vector x along $E^{\perp}$ as is illustrated in Fig. 3 with an example in two dimensions which reproduces the situation in four dimensions where we are interested in the intersection of $E^{\parallel}$ with two-dimensional facets of the hypercube. By calculating the angle between $E^{\parallel}$ and one basis vector of $\mathcal{L}$, after a straightforward trigonometric calculation, one gets that if $x = \sum_{i=1}^{4} \mathrm{round}(l_1^{\parallel} \cdot e_i)e_i = \sum_{i=1}^{4} \mathrm{round}(l_2^{\parallel} \cdot e_i)e_i$, then

$$||x^{\perp}|| \leq \tfrac{1}{2}\cos(2\theta)/[1 + (\cos 2\theta)^2]^{1/2}. \qquad (10)$$

This defines a cylindrical 'pipe' instead of the standard strip considered in the cut and projection method. The projection onto $E^{\parallel}$ of x yields the best-fit point between $l_1^{\parallel}$ and $l_2^{\parallel}$.

In short, the projection onto $E^{\parallel}$ of all the vertices $x \in \mathcal{L}$ that fulfil the condition (10) defines $\mathcal{G}$, the set of points of good fit between L_1 and L_2, *i.e.* the GCSN. Observe that this is in general a subset of that obtained by the standard cut and projection method, which

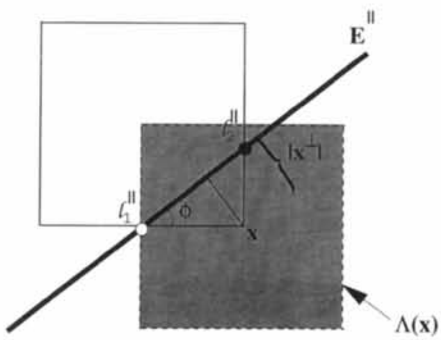


Fig. 3. Two-dimensional example of the situation in which two vertices $l_1^{\parallel} \in L_1$ and $l_2^{\parallel} \in L_2$ lie in a Voronoi cell. In such a case, we have $x = \sum_{i=1}^{2} \mathrm{round}(l_1^{\parallel} \cdot \mathbf{e}_i)\mathbf{e}_i = \sum_{i=1}^{2} \mathrm{round}(l_2^{\parallel} \cdot \mathbf{e}_i)\mathbf{e}_i$. The value of $||x^{\perp}||$ can be calculated easily if we know the angle between $E^{\parallel}$ and one edge of the square.

additionally projects the vertices of $\mathcal{L}$ (centers of Voronoi cells) that lie inside the strip. Clearly, many of these centers correspond to points $l_1^{\parallel}$ and $l_2^{\parallel}$ that do not fulfil the conditions (9) or (10).

4. Non-eutactic stars

In the previous discussion, it was assumed that the embedding (7) exists, which means that the grid g can be viewed as the intersection of $E^{\parallel}$ with a four-dimensional cubic grid G. This is true for the example of the two rotated square lattices discussed here since the star defined by $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4\}$ is eutactic for any value of θ [for the eutacticity criterion, see Coxeter (1973) and Gómez, Aragón & Dávila (1991)]. This means that there exists a four-dimensional orthonormal set $\{e_1, e_2, e_3, e_4\}$ such that $\mathbf{a}_i = P^{\parallel}(e_i)$, $i = 1, \ldots, 4$, where $P^{\parallel}$ is the projector from $\mathbf{R}^4$ to $E^{\parallel}$. For a general star $\{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_6\}$ defining two lattices L_1 and L_2, this is no longer true. In this case, it is possible that there is no n-dimensional embedding in which g can be viewed as the intersection of a cubic grid in n dimensions, making it necessary to consider noncubic lattices (Gómez, Aragón & Dávila, 1991).

This might be important when one is interested in the use of the cut and projection method to obtain the set of good-fit points between two arbitrary lattices, which, furthermore, can be of different density. The higher-dimensional formulation of this general case is not trivial, however we can give some clues on how to achieve this.

The first thing one needs is to find a procedure to correctly embed the space of the grid, $E^{\parallel}$, in $\mathbf{R}^6$. It is completed once we define the projector $P^{\parallel} : \mathbf{R}^6 \to E^{\parallel}$ such that $E^{\parallel}$ be the range of $P^{\parallel}$. In what follows, we propose a general method to find this projector for the case of two arbitrary three-dimensional lattices generated by $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ and $\{\mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6\}$, respectively. In this case, the grid g generated by the star $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6\}$ will be viewed as the intersection with a six-dimensional grid G whose intersection points define a noncubic six-dimensional lattice $\mathcal{L}$. The projector $P^{\parallel}$ and the metric tensor of $\mathcal{L}$ will be defined.

Let $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$, $\{\mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6\}$, $\{\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*\}$ and $\{\mathbf{a}_4^*, \mathbf{a}_5^*, \mathbf{a}_6^*\}$ be as before, then, since for every $\mathbf{x} \in \mathbf{R}^3$

$$\mathbf{x} = \sum_{i=1}^{3}(\mathbf{x} \cdot \mathbf{a}_i^*)\mathbf{a}_i = \sum_{i=4}^{6}(\mathbf{x} \cdot \mathbf{a}_i^*)\mathbf{a}_i,$$

it follows that

$$\mathbf{x} = \tfrac{1}{2}\sum_{i=1}^{6}(\mathbf{x} \cdot \mathbf{a}_i^*)\mathbf{a}_i.$$

Defining $\mathbf{b}_i^* = \mathbf{a}_i^*$ and $\mathbf{b}_i = \mathbf{a}_i/2$, we have

$$\mathbf{x} = \sum_{i=1}^{6}(\mathbf{x} \cdot \mathbf{b}_i^*)\mathbf{b}_i$$

and this expression has the form required in the generalized Hadwiger theorem (Gómez, Aragón & Dávila, 1991) so there exists a basis $\{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_6\}$ of $\mathbf{R}^6$ (not necessarily orthonormal) with reciprocal basis $\{\varepsilon_1^*, \varepsilon_2^*, \ldots, \varepsilon_6^*\}$ and such that $P^{\parallel}(\varepsilon_i) = \mathbf{b}_i$ and $P^{\parallel}(\varepsilon_i^*) = \mathbf{b}_i^*$. The matrix elements of this projector can be shown to be given by

$$P_{i,j}^{\parallel} = \mathbf{b}_i^* \cdot \mathbf{b}_j.$$

The metric tensor (Gram matrix) of the basis in $\mathbf{R}^6$ can be obtained unambiguously if the extra condition is imposed that the subspaces of $\mathbf{R}^6$ from which $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ and $\{\mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6\}$ project are mutually orthogonal. Then the metric tensor becomes

$$g_{k,j} = \mathbf{a}_k \cdot \mathbf{a}_j/2.$$

5. Rational approximants and coincidence lattices

Here we shall point out the relationship between the so-called rational approximants (Goldman & Kelton, 1993) and coincidence lattices. To this end, we turn back to the example of the two square lattices developed in §3, considering the cut and projection method.

In this higher-dimensional approach, a change in the value of the angle θ between L_1 and L_2 is equivalent to a rotation of the strip, which, depending on the value of $\tan\theta$, can be rational or irrational with respect to $\mathcal{L}$. For irrational values of $\tan\theta$, the best-fit lattice is a quasiperiodic structure and, for rational orientations, it is a rational approximant of the quasiperiodic lattice.

There are several ways to obtain periodic structures using the cut and projection method (Yacamán & Torres, 1993). The most suitable for our purposes considers that the change of the angle θ induces a distortion of the lattice $\mathcal{L}$ along $E^{\perp}$, the space perpendicular to $E^{\parallel}$, yielding a distorted lattice $\tilde{\mathcal{L}}$ from which rational approximants can be obtained by cut and projection. Since the projection onto the physical space remains unchanged, the tiles preserve their shape but become rearranged to form a periodic structure.

Let us return to our two-dimensional example and consider the two lattices L_1 and L_2 generated by $\{\mathbf{a}_1, \mathbf{a}_2\}$ and $\{\mathbf{a}_3, \mathbf{a}_4\}$ given by equation (6) and shown in Fig. 1. If $\theta = 22.5°$, we have that $\tan\theta = 1/(1 + 2^{1/2})$ and the star $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4\}$ points to four vertices of an octagon. The four basis vectors of $\mathbf{R}^4$ project onto equation (6) and the GCSN between L_1 and L_2 is a subset of the octagonal quasiperiodic tiling.

For rational orientations, say $\tan\theta = p/q$, the distorted lattice $\tilde{\mathcal{L}}$ has nonzero intersections with $E^{\parallel}$ ($E^{\parallel}$ is actually a lattice plane of $\tilde{\mathcal{L}}$) and, therefore, projection produces a periodic structure. The set points of $\tilde{\mathcal{L}}$ intersecting $E^{\parallel}$ is the CSL between L_1 and L_2. In other words, the CSL is the set of points of $\tilde{\mathcal{L}}$ with zero component along $E^{\perp}$. The deformed lattice $\tilde{\mathcal{L}}$ can be obtained by considering that $\mathcal{L}$ can be written, in a rotated basis, as the integer linear combination of the vectors

$$\begin{aligned}
\varepsilon_1 &= 2^{-1/2}(\cos\theta, \sin\theta, -\sin\theta, \cos\theta),\\
\varepsilon_2 &= 2^{-1/2}(-\sin\theta, \cos\theta, -\cos\theta, -\sin\theta),\\
\varepsilon_3 &= 2^{-1/2}(\cos\theta, -\sin\theta, -\sin\theta, -\cos\theta),\\
\varepsilon_4 &= 2^{-1/2}(\sin\theta, \cos\theta, \cos\theta, -\sin\theta),
\end{aligned} \tag{11}$$

where the last two components of each vector are the projection of the basis vectors (or $\mathbf{R}^4$) onto $E^{\perp}$.

Now we shall deform the components of equation (11) along $E^{\perp}$ to obtain a lattice $\tilde{\mathcal{L}}$ commensurate with $E^{\parallel}$. This can be performed by writing $\cos\theta$ and $\sin\theta$ in terms of $\tan\theta = p/q$ in the $E^{\perp}$ components of (11) and, in order to preserve the projections onto $E^{\parallel}$, we take $\theta = \theta_{qc} = 22.5°$ for the parallel components. This gives the set

$$\begin{aligned}
\tilde{\varepsilon}_1 &= 2^{-1/2}\left(\cos\theta_{qc}, \sin\theta_{qc}, -\frac{p}{(p^2+q^2)^{1/2}}, \frac{q}{(p^2+q^2)^{1/2}}\right),\\
\tilde{\varepsilon}_2 &= 2^{-1/2}\left(-\sin\theta_{qc}, \cos\theta_{qc}, -\frac{q}{(p^2+q^2)^{1/2}}, -\frac{p}{(p^2+q^2)^{1/2}}\right),\\
\tilde{\varepsilon}_3 &= 2^{-1/2}\left(\cos\theta_{qc}, -\sin\theta_{qc}, -\frac{p}{(p^2+q^2)^{1/2}}, -\frac{q}{(p^2+q^2)^{1/2}}\right),\\
\tilde{\varepsilon}_4 &= 2^{-1/2}\left(\sin\theta_{qc}, \cos\theta_{qc}, \frac{q}{(p^2+q^2)^{1/2}}, -\frac{p}{(p^2+q^2)^{1/2}}\right),
\end{aligned} \tag{12}$$

so that $\tilde{\mathcal{L}} = \{l \in \mathbf{R}^4 | l = \sum_{i=1}^4 n_i\tilde{\varepsilon}_i, \quad n_i \text{ integers}\}$. The CSL, L_{csl}, is the intersection of $E^{\parallel}$ with $\tilde{\mathcal{L}}$, that is, the set of points $l \in \tilde{\mathcal{L}}$ with zero component along $E^{\perp}$. By doing this in equation (12), we can find a basis $\{\mathbf{b}_1, \mathbf{b}_2\}$ for L_{csl} that, after solving a diophantine system, yields

$$\begin{aligned}
\mathbf{b}_1 &= 2^{1/2}(q\cos 22.5 + p\sin 22.5, 0),\\
\mathbf{b}_2 &= 2^{1/2}(0, q\cos 22.5 + p\sin 22.5)
\end{aligned}$$

if $(p+q)/2 \notin Z$. Otherwise, the basis is $\{(\mathbf{b}_1+\mathbf{b}_2)/2, (\mathbf{b}_2-\mathbf{b}_1)/2\}$.

This last result gives us a general expression for the basis vectors of the CSL for a given angle between the lattices such that $\tan\theta = p/q$.

6. Examples

As an example, we have calculated some structures obtained by the cut and projection method following the criterion (10) for two square lattices. Fig. 4 shows the GCSN structure corresponding to a quasiperiodic lattice obtained for $2\theta = 45°$, with 2θ being the angle between L_1 and L_2. This tiling is a subset of the standard octagonal quasiperiodic tiling. Following the notation used in the grain-boundaries field, Figs. 5(*a*) to (*c*) show the structures corresponding to $\Sigma 5$ ($2\theta = 36.87°$), $\Sigma 13$ ($2\theta = 22.62°$) and $\Sigma 17$ ($2\theta = 28.07°$), respectively, all containing the associated CSL, whose primitive cells are shaded.

7. Conclusions

In this work, the problem of finding the points of good fit between pairs of lattices was solved using a higher-dimensional approach through a modified version of the cut and projection method. The good-fit criterion was provided by the GCSN method, which has been shown to describe accurately several general properties of grain boundaries. The formalism was presented in detail for the particular case of two square lattices rotated by an angle θ and it was shown that the problem is equivalent to cut and projection with the usual strip replaced by a cylindrical 'pipe'.

Making use of the fact that a change in the misorientation angle θ corresponds to a rotation in higher-dimensional space, a description of the CSL of two square lattices and a prescription to find its basis vectors in terms of the angle θ were given. A connection was also established between the best-fit

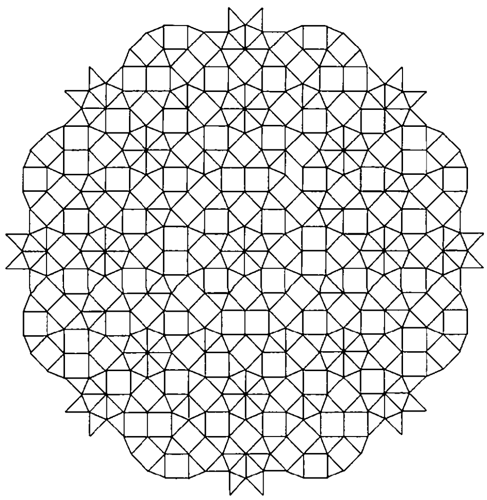
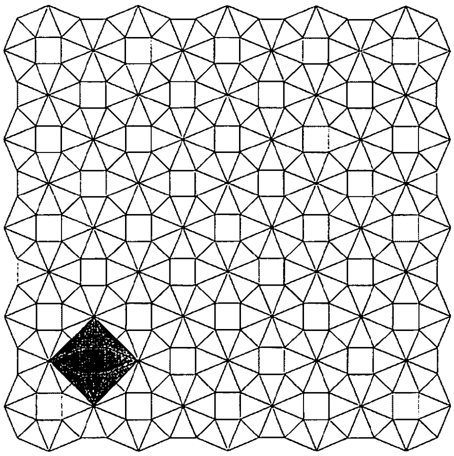
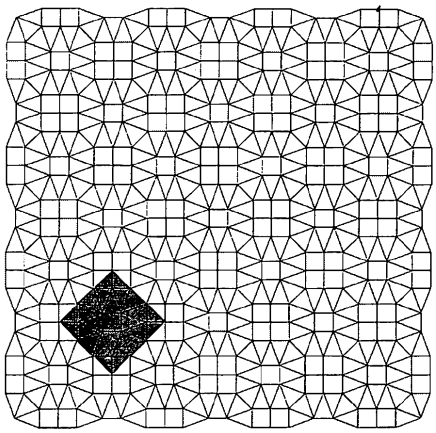


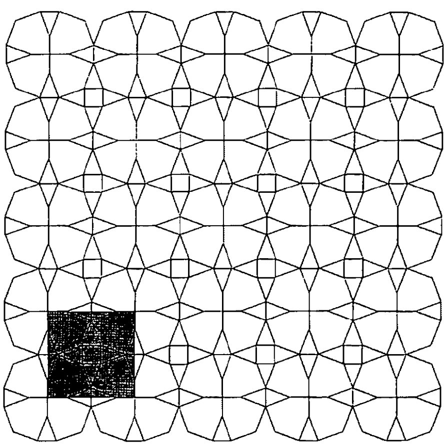
Fig. 4. The best-fit lattice (GCSN) of two square lattices with $2\theta = 45°$ obtained by the cut and projection method. It is a subset of the octagonal quasiperiodic tiling.



(a)



(b)



(c)

Fig. 5. The best-fit lattice (GCSN) of two square lattices with special orientations according the terminology used in grain boundaries. (a) $\Sigma 5$ ($2\theta = 36.87°$), (b) $\Sigma 13$ ($2\theta = 22.62°$) and (c) $\Sigma 17$ ($2\theta = 28.07°$). The primitive cells of the CSL associated with each structure are shaded.

lattice and the rational approximants of quasiperiodic structures.

Viewing grain boundaries as projections of lattices from higher dimensions provides a fruitful insight into both fields. Our calculations were performed in two dimensions where the connection with the cut and projection method is clearer. The extension to three dimensions for simple cubic lattices is straightforward. The case of more general lattices (which includes the case of lattices with different density) might not be trivial. In §4, some tools that can help in this last case are presented.

This work was supported by CONACyT through grants 0205P-E9506, 0088P-E and 5165-E and DGAPA (UNAM) through grants IN-104296 and IN-107296.

References

Bishop, G. H. & Chalmers, B. (1968). *Scr. Metal.* **2**, 133–140.

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

Bollmann, W. (1982). *Crystal Lattices, Interfaces, Matrices. An Extension of Crystallography*. Geneva: W. Bollmann.

Bruijn, N. G. de (1981). *Ned. Akad. Wet. Proc. Ser. A*, **43**, 39–66.

Conway, J. H. & Sloane, N. J. A. (1988). *Sphere Packings, Lattices and Groups*, ch. 20. New York: Springer-Verlag.

Coxeter, H. S. M. (1973). *Regular Polytopes*, Section 13.7. New York: Dover.

Duneau, M. & Katz, A. (1985). *Phys. Rev. Lett.* **54**, 2688–2691.

Gähler, F. & Rhyner, J. (1986). *J. Phys. A: Math. Gen.* **19**, 267–277.

Galiulin, R. V. (1980). *Sov. Phys. Crystallogr.* **25**, 517–520.

Goldman, A. I. & Kelton, K. F. (1993). *Rev. Mod. Phys.* **65**, 213–230.

Gómez, A., Aragón, J. L. & Dávila, F. (1991). *J. Phys. A: Math. Gen.* **24**, 493–500.

Gómez, A., Beltrán, L., Aragón, J. L. & Romeu, D. (1997). *Acta Metall.* Submitted.

Gratias, D. & Thalal, A. (1988). *Philos. Mag. Lett.* **57**, 63–68.

Kramer, P. & Neri, R. (1984). *Acta Cryst.* A**40**, 580–587.

Levine, D. & Steinhardt, P. J. (1986). *Phys. Rev. B*, **34**, 596–616.

Ranganathan, S. (1966). *Acta Cryst.* **21**, 179–199.

Rivier, N. & Lawrence, A. (1988). *Physica (Utrecht)*, B**150**, 190–202.

Romeu, D., Beltrán, L., Aragón, J. L. & Gómez, A. (1997). *New Horizons in Quasicrystals: Research and Applications*, edited by A. Goldman, D. Sordelet, P. Thiel & J. M. Dubois, pp. 119–126. Singapore: World Scientific.

Smith, D. A. & Pond, R. C. (1976). *Int. Met. Rev.* **205**, 61–74.
Sutton, A. P. (1988). *Acta Metall.* **36**, 1291–1299.
Yacamán, M. J. & Torres, M. (1993). Editors. *Crystal–Quasicrystal Transitions*. Amsterdam: Elsevier.