Interfaces and quasicrystals as competing crystal lattices: Towards a crystallographic theory of interfaces

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This paper shows that in a higher-dimensional approach, quasicrystals and interfaces are formally equivalent. Interfaces and quasicrystals are interpreted here as a region in space where the atoms of interpenetrated crystal lattices compete for space. Based on this paradigm, a method derived from the strip-projection method developed for the study of quasicrystals has been introduced. The method is completely general, independent of the parent crystal lattice type, relative orientation, and translation and of the position and orientation of the boundary plane. In this approach the perpendicular space coincides with Bollmanns' displacement space, while the parallel space contains a physical structure characterized by a minimum local strain that includes both the interface and adjacent crystal lattices. A classification of interfaces in a finite number of well-defined equivalence classes (local isomorphisms) that include orientational and translational degrees of freedom has been introduced. This classification is based on the symmetry of the hyperlattice and the position and shape of the strip and incorporates concepts from previous structural units and symmetry breaking approaches. It is suggested that such classes can be related to physical properties of interfaces. The formalism defines ideal (minimum strain) structures assumed to play an analogous role in grain boundaries (GB's) to those played by the perfect crystal and quasicrystal concepts in the study of crystals and quasiperiodic structures. Also, a lattice, called the phason lattice, is introduced to account for the dislocation content of nonsingular interfaces. Accordingly, the properties of any GB are seen to be determined by the periodicity of isosymmetrical regions related to the O and phason lattices and not by the ill-defined and pathologically discontinuous index number Σ.

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I. INTRODUCTION

In spite of its technological importance, there is at present no general theory of interfaces capable of relating the physical properties of general grain boundaries (GB's) to their structure. Since it is well known that different boundaries have different properties, a large amount of work has been devoted to the creation of a classification scheme that would allow the grouping of GB's into a hopefully finite number of (property-related) classes, equivalent to the Bravais lattices of crystals. When studying the properties of crystals, the first thing that is specified is the lattice type (space group), followed by an analysis of the existing defects or alterations of the ''perfect lattice'' that may account for the observed properties. Unfortunately, this procedure cannot be used for interfaces since there are no ideal (defect-free) reference structures to compare with, making it difficult to ascertain whether a given property is due to an intrinsic interfacial feature or to an extrinsic defect. If the study of interfaces is to have a similar degree of success to that of crystals, the development of a crystallography of interfaces is needed.

Among the numerous efforts to classify interfaces, the works of Pond and co-workers[1,2] (see the book by Sutton and Balluffi[3] for a detailed account) and Vitek and Sutton[4] deserve special mention. These authors have approached the problem of interfacial characterization from the complementary points of view of (a) symmetry—based on group theoretical considerations—and (b) structure—based on an analysis of the content and distribution of structural units obtained from computer simulations. Each from their own perspective has introduced fundamental ideas to the field, such as symmetry variants and the concept of delimiting (special) and intervening (general) boundaries. Nevertheless, GB's are still crudely classified in the practice into three broad classes[5]: (a) low-angle, (b) special or singular, and (c) general boundaries, which bear little relation to structure.

The purpose of this paper is to show that by regarding interfaces as the projection onto the three-dimensional (3D) space of a suitable defined higher-dimensional hyperlattice, we find a new classification of interfaces in well-defined equivalence classes that include orientational and translational degrees of freedom that incorporates the results of the above classification schemes and provides an important step towards the formulation of a general crystallographic theory for interfaces. It will be shown that interfaces and quasicrystals are formally equivalent in the sense that they can be described by the same set of equations and that these equations can be used to define an ideal or ''perfect interface,'' in analogy with the concepts of ''perfect quasicrystal'' and ''perfect crystal.'' The higher-dimensional (HD) approach provides the mathematical background needed to define unambiguously delimiting and intervening interfaces as well as the dependence and evolution of the symmetry variants with the macroscopic and microscopic degrees of freedom that define an interface.

The possibility of using a higher-dimensional approach to study interfaces was first realized by Gratias and Thalal[6] who used it to study general characteristics of interfaces. Also, Warrington *et al.*[7] have used it to investigate the properties of interfaces between nonperiodic crystals (quasicrystals). The first attempt to describe in some detail the geometry of

general every day GB's was made by Aragón *et al.*[8] using the conventional method of starting out with a predefined hyperlattice. Unfortunately, this limits the usefulness of the method by preventing it from dealing with symmetry variants. This limitation is remedied in this work by letting the hyperlattice symmetry vary with the relative orientation (and symmetry) of the parent crystals (see Sec. IV).

Although at first sight it may appear that introducing extra dimensions into the problem complicates the issue unnecessarily, it actually makes it simpler. For example, it is easier to envisage (both conceptually and mathematically) the crystallographic properties of a single crystal in 6D than those of a dichromatic pattern (two interpenetrated lattices in 3D), which is cumbersome to handle, difficult to visualize, and requires the introduction of color symmetry groups. Additionally, the symmetry changes (orientational and translational variants[2]) of dichromatic patterns arising from variations in the rotational and translational degrees of freedom are difficult to follow in detail using conventional methods. In the HD approach, the evolution of orientational and translational variants can be easily followed since the method decouples these degrees of freedom, allowing them to be studied separately. Orientational variants or, more precisely, local isomorphisms[9] depend only on the symmetry of the hyperlattice which depends on the symmetry and orientation of the parent crystals and is unaffected by relative displacements. Translational variants, in turn, are described by displacements of the strip (see Sec. IV) in a direction orthogonal to the physical space, leaving the hyperlattice symmetry intact. It will also be shown that the number of rotational and translational variants is denumerable (and effectively finite), significantly simplifying the characterization task.

Given a completely arbitrary set of degrees of freedom, the HD approach provides explicit analytical expressions that produce an interfacial lattice (or quasilattice) that minimizes the local strain everywhere. Since it is sensible to assume that, to a first approximation, actual interfaces also minimize local strain in order to minimize elastic energy, it is argued that this lowest strain (best fit) structure defines the needed defect-free reference structure or ''perfect interface'' suitable for characterization purposes. Actually, the method produces a complete bicrystal; i.e., it gives not only the points at the interface, but also those of the adjacent crystals.

One fundamental property of the method is its generality. It does not depend on lattice type, relative orientation, and translation of the parent crystals or on the orientation and location of the boundary plane. Also, it introduces the concept of ''phason,'' which appears naturally in a HD context into the theory of interfaces. As we shall see, phason defects are required for a complete understanding of the geometrical aspects of interfaces. The approach has already shown its usefulness by accounting for the extra O points found in low-angle 110-twist GB's (Ref. 10) through the GCSN model,[11] which is a corollary of the HD approach.

In the following sections, the formalism will be developed in all generality and it will be illustrated using the results of the GCSN model for rotation related interfaces[12] which corresponds to a particular choice of strip (see Sec. IV). The lattices needed to describe interfaces will be formulated in this context and a new lattice shall be introduced called phason lattice or P lattice for short.

II. PERIODIC VERSUS NONPERIODIC INTERFACES

It is important to realize that, in practice, all interfaces can be regarded as periodic. For any irrational orientation between two lattices (resulting in a nonperiodic interface) and within *any* degree of accuracy, there exists an infinite number of rational orientations corresponding to periodic, coincidence GB's (CGB's). The same reasoning applies to epitaxial interfaces between crystals with ''incommensurate'' unit cells. Therefore, with no loss of generality, all GB's can be considered as periodic, albeit of an arbitrarily large period.

Every periodic GB is associated with a coincidence site lattice (CSL) characterized by its index number Σ, numerically equal to the reciprocal of the density of coincidence sites. Σ is a pathologically discontinuous function of the misorientation angle: an infinitesimal change in the latter can result in an arbitrarily large change in Σ. Since one expects physical properties to be continuous, no physical property can be a continuous function of Σ, so that its use as a classification criterion is doomed to failure. In spite of this, it is often used to describe or at least label interfaces. Consider for example the case of the so-called special or singular GB's (Ref. 13); it is customary to assume that singular GB's are short period CGB's (small Σ). Now consider the case of low-angle GB's and its network of primary dislocations.[14] In such boundaries, the dislocation density and hence the interfacial energy decrease continuously with decreasing misorientation angle θ until they vanish at $\theta=0$, but Σ (the GB period) increases without limit as $\theta\rightarrow 0$. Therefore the interfacial energy actually increases with decreasing Σ, in contradiction with the usual assumption, an inconsistency usually bypassed by considering low-angle GB's as belonging to a class of their own.[5]

It has been recently proposed[12] that singular CGB's, hereafter called ''delimiting'' (DGB's) after Vitek and Sutton,[4] are mathematically characterized by a zero deviation parameter δ [see Eq. (19)]. All DGB's contain primary dislocations with crystalline Burgers vectors. All other CGB's, characterized by a nonzero deviation parameter, are called intervening GB's (IGB's) and contain dislocations with noncrystalline Burgers vectors.

III. INTERFACIAL LATTICES

Since a number of lattices in three and six dimensions are needed to introduce the method, a note on notation is needed at this point. In what follows, an n-dimensional lattice Λ will be represented by an expression of the form $\Lambda=\hat{\mathbf{L}}\mathbf{B}\mathbf{Z}^{(n)}$ where $\mathbf{B}$ is the (identity) matrix whose columns are the vectors of the standard orthonormal basis endowed with units of distance and $\mathbf{Z}^{(n)}$ is an n-dimensional $\mathbf{Z}$ modulus (the set of integral column vectors in n dimensions). The need for setting the units aside into $\mathbf{B}$ will become clear when discussing the difference between perpendicular and reciprocal spaces. $\hat{\mathbf{L}}$ represents the (dimensionless) structure matrix of the lattice and will often be written as the product $\hat{\mathbf{L}}=\mathbf{T}\mathbf{L}$ with $\mathbf{L}$

being the transformation that brings the orthonormal basis into the unit vectors of a specified (Bravais) lattice and **T** any further operation needed to reorient or deform the lattice such as a rotation, shear, or expansion.

Given two completely arbitrary lattices $\mathbf{\Lambda}_1=\hat{\mathbf{L}}_1\mathbf{BZ}^{(n)}$ and $\mathbf{\Lambda}_2=\hat{\mathbf{L}}_2\mathbf{BZ}^{(n)}$ there exists a transformation **T** such that $\mathbf{\Lambda}_1=\mathbf{T}\mathbf{\Lambda}_2$. It will be convenient to work in terms of the median lattice $\mathbf{\Lambda}_m$ where equations are more symmetrical and aesthetically pleasant. The median lattice lies ''halfway'' between $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$ and is defined by

$$\mathbf{\Lambda}_m=\mathbf{L}_m\mathbf{BZ}^{(n)}=(\mathbf{M}\hat{\mathbf{L}}_1)\mathbf{BZ}^{(n)}, \tag{1}$$

with **M** being the minimum norm matrix such that $\mathbf{M}^2=\mathbf{T}$. Clearly $\hat{\mathbf{L}}_m=\mathbf{L}_m=\mathbf{M}\hat{\mathbf{L}}_1=\mathbf{M}^{-1}\hat{\mathbf{L}}_2$. For simplicity, in what follows we shall refer to a lattice using either Λ, $\hat{\mathbf{L}}$, or **L** as found convenient. Note the median lattice is preferred simply because of the symmetry of the equations.

In order to describe an arbitrary interface we shall need two lattices: the O lattice (**O**) and the P lattice (**P**), all other lattices being derivable from these. The **O** and **P** lattices play equivalent roles for DGB's and IGB's; namely, they respectively describe the primary and nonprimary dislocation content of DGB's and IGB's.

Other important lattices are the coincidence sites lattice (CSL) **C** which is a sublattice of **O**, the secondary O lattice **S** which is a sublattice of **P**, and the DSC lattice **D**, defined as the set of vectors joining the points of the two lattices. As will become clear below, **O** and **C** are physically meaningful only for DGB's; when dealing with IGB's, they must be replaced by their equivalent **P** and **S** lattices. Since interfacial points are arranged in domains defined by the dislocation network and domains may have different symmetries,[12] the lattices $\mathbf{U}_i$, $i=1,n$, are needed to specify the atomic arrangements (structural units) within each of the n domain types of an interface.

All lattices above are defined in the physical 3D space denoted $\mathbf{E}^{\|}$ and called parallel space. A related set of lattices appears in the orthogonal complement of $\mathbf{E}^{\|}$ called ''perpendicular space'' represented by $\mathbf{E}^{\perp}$. The lattices in $\mathbf{E}^{\perp}$ are defined by structure matrices given by the inverse transpose of their (dimensionless) $\mathbf{E}^{\|}$ counterparts. $\mathbf{E}^{\perp}$ lattices play a vital role in the characterization of interfaces since they constitute a reduced representation of the displacement field at the interface and can be used to calculate the diffraction properties of interfaces. For clarity, their description shall be deferred to a second publication dealing with the structure of $\mathbf{E}^{\perp}$ and the diffraction properties of interfaces.

IV. MODIFIED STRIP-PROJECTION METHOD

The method presented here consists of a modified version of the strip method of Katz and Duneau[15,16] devised to study the crystallographic properties of quasicrystals. The main difference with the original strip method resides in that, there, a high-symmetry (normally cubic) hyperlattice is sought at the onset such that its unit vectors project onto a set of six linearly dependent vectors (a star vector) in the 3D physical space. The star vector has the point symmetry of the quasicrystal but it is not otherwise related to its structure. The end result of this procedure is a (nondecorated) tiling describing the geometry of quasicrystals and interfaces,[8] but with no detailed structural information. This limitation is overcome by defining the hyperlattice $\mathbf{\Lambda}^{(6)}$ as the Cartesian product of the interpenetrated 3D crystal lattices $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$ embedded in a 6D space. As a result, the structure of $\mathbf{\Lambda}^{(6)}$ is completely determined by $\mathbf{\Lambda}_1,\mathbf{\Lambda}_2$ and the transformation relating them. Also, the base vectors of $\mathbf{\Lambda}^{(6)}$ project into the base vectors of $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$. This links the structures of $\mathbf{\Lambda}^{(6)}$, $\mathbf{\Lambda}_1$, and $\mathbf{\Lambda}_2$, allowing the method to produce an actual interfacial lattice in real space, at the expense of a reduction of the hyperlattice symmetry. The rest of the process remains basically identical to the original.

To avoid atomic overlap, only those hyperlattice points falling within a bounded region around $\mathbf{E}^{\|}$ called the strip are projected (see Fig. 1). The strip selects hyperpoints with small associated strain or frustration (Sec. IV B) and its shape depends upon the symmetries of $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$ and the nature of atomic interactions. Once the strip is specified, it is possible to model not only the interface but a complete bicrystal as shown in Fig. 1.

A. Ideal interfaces vs perfect crystals

The modified strip-projection produces ideal 3D structures characterized by a minimum local strain between nearest neighbors at the interface (see below). An ideal interface is a concept equivalent to that of a perfect crystal. Decorated Bravais lattices are used to characterize real crystals in spite of the fact that they do not include dislocations, vacancies, and other defects that are known to exist in real crystals. This is because they provide a clear and mathematically manageable picture of the underlying geometry and allow real crystals to be understood in terms of their differences from an ideal lattice by analyzing diffraction data. Analogously, although some differences are expected between ideal and real interfaces, it is the contention of this paper that ideal interfaces can be used to build a crystallographic description of interfaces. That this is indeed the case is demonstrated by the quantitative agreement obtained with experimental observations on fcc twist interfaces, as described below.

Ideal interfaces are expected to represent better those systems which minimize energy mostly through strain minimization (as expected from systems with largely isotropic interatomic potentials). Of course, some differences are expected between ideal and real interfaces, but as for crystals, by analyzing these differences through diffraction data, an insight into the mechanisms controlling the structure of real interfaces can be gained. Also, ideal interfaces can always be used as a first-order initial configuration to be refined by computer simulations. This information can later be fed back into the formalism to provide a more exact description of the geometry of particular systems. This will introduce system-dependent relaxational variants,[1,2] but the ideal prerelaxed structure is still useful from a crystallographic point of view, just as normal Bravais lattices.

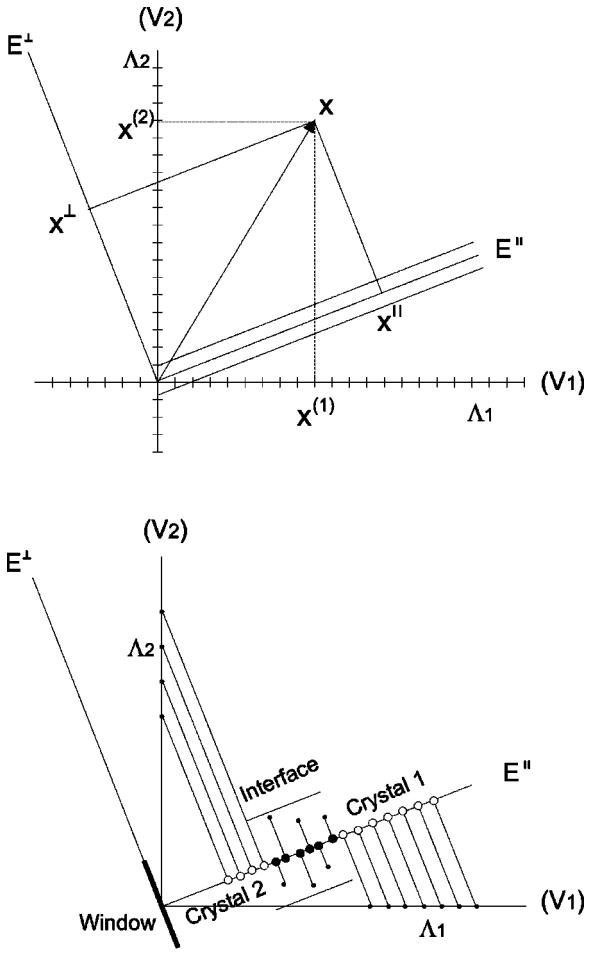

FIG. 1. Schematic representation of the projection of a 2D hyperlattice into the 1D orthogonal subspaces $\mathbf{E}^{\parallel}$ and $\mathbf{E}^{\perp}$. Top: the hyperpoint point $\mathbf{x}$ results from the embedding of the lattice points $\mathbf{x}^{(1)},\mathbf{x}^{(2)}$ and projects onto the points $\mathbf{x}^{\parallel},\mathbf{x}^{\perp}$. Only points within the region around $\mathbf{E}^{\parallel}$ bounded by the strip are projected. Bottom: the projection of a complete bicrystal: interfacial points arise from the projection of the hyperpoints inside the strip that lie within the region of conflict. Crystals 1 and 2 are recovered by projecting the hyperpoints $(\mathbf{x}^{(1)},0)$ and $(0,\mathbf{x}^{(2)})$.

B. Six-dimensional hyperlattice

Letting $\hat{\mathbf{L}}_1$, $\hat{\mathbf{L}}_2$ be the structure matrices of two crystal lattices $\mathbf{\Lambda}_1$, $\mathbf{\Lambda}_2$, the hyperlattice is defined (in the canonical basis of $\mathbf{R}^6$) by the structure matrix $\mathbf{L}_m^{(6)}$ given by

$$\mathbf{L}_m^{(6)}=\sqrt{2}\begin{pmatrix}\hat{\mathbf{L}}_1 & 0\\ 0 & \hat{\mathbf{L}}_2\end{pmatrix}. \tag{2}$$

The first and last three columns of $\mathbf{L}_m^{(6)}$ span two orthogonal 3D subspaces $\mathbf{V}_1$, $\mathbf{V}_2$ of $\mathbf{R}^6$ and generate the crystal lattices $\hat{\mathbf{L}}_1$, $\hat{\mathbf{L}}_2$ (expanded by $\sqrt{2}$) in the disjoint subspaces $\mathbf{V}_1,\mathbf{V}_2$ where they no longer compete for space (see Fig. 1). The $\sqrt{2}$ expansion is needed for proper projection[17] but is irrelevant to the physics of the problem and can be ignored, so that $\mathbf{L}_m^{(6)}$ is simply the Cartesian product $\hat{\mathbf{L}}_1\otimes\hat{\mathbf{L}}_2$.

Since $\mathbf{V}_1$ and $\mathbf{V}_2$ are orthogonal, $\mathbf{R}^6$ and $\mathbf{\Lambda}^{(6)}$ are given by the direct sums $\mathbf{R}^6=\mathbf{V}_1\oplus\mathbf{V}_2$ and $\mathbf{\Lambda}^{(6)}=\mathbf{\Lambda}_1\oplus\mathbf{\Lambda}_2$. The decisive step consists in realizing that $\mathbf{R}^6$ is also given by the direct sum $\mathbf{R}^6=\mathbf{E}^{\parallel}\oplus\mathbf{E}^{\perp}$. Therefore, any hyperlattice point $\mathbf{x}$ can be written (disregarding the $\sqrt{2}$ factor) as an ordered pair in two different bases $\mathbf{x}=(\mathbf{x}^{(1)},\mathbf{x}^{(2)})=(\mathbf{x}^{\parallel},\mathbf{x}^{\perp})$ with $\mathbf{x}^{(1)}\in\mathbf{\Lambda}_1$, $\mathbf{x}^{(2)}\in\mathbf{\Lambda}_2$, $\mathbf{x}^{\parallel}\in\mathbf{E}^{\parallel}$, and $\mathbf{x}^{\perp}\in\mathbf{E}^{\perp}$. Note $(\mathbf{x}^{(1)},\mathbf{x}^{(2)})$ and $(\mathbf{x}^{\parallel},\mathbf{x}^{\perp})$ refer to the same hyperpoint expressed in the coordinate systems of $(\mathbf{\Lambda}_1,\mathbf{\Lambda}_2)$ and $(\mathbf{E}^{\parallel},\mathbf{E}^{\perp})$.

The $\mathbf{x}^{\parallel}$ component of $\mathbf{x}$ is given by $\mathbf{\Pi}(\mathbf{x})$ where $\mathbf{\Pi}$ is an orthogonal projector given by the block matrix

$$\mathbf{\Pi}=\frac{1}{2}\begin{pmatrix}\mathbf{I} & \mathbf{I}\\ \mathbf{I} & \mathbf{I}\end{pmatrix}, \tag{3}$$

and $\mathbf{I}$ is the identity matrix in 3D. The perpendicular space component $\mathbf{x}^{\perp}$ is in turn given by $\mathbf{\Pi}^{\perp}(\mathbf{x})$ with $\mathbf{\Pi}^{\perp}=\mathbf{I}-\mathbf{\Pi}$. Using Eq. (3) we obtain two fundamental equations

$$\mathbf{x}^{\parallel}=\mathbf{\Pi}(\mathbf{x})=\frac{1}{2}(\mathbf{x}^{(1)}+\mathbf{x}^{(2)}), \tag{4}$$

$$\mathbf{x}^{\perp}=\mathbf{\Pi}^{\perp}(\mathbf{x})=\frac{1}{2}(\mathbf{x}^{(1)}-\mathbf{x}^{(2)}). \tag{5}$$

Since $\mathbf{x}$ must be contained in the strip, the latter is chosen to include the pair of atoms at $\mathbf{x}^{(1)},\mathbf{x}^{(2)}$ occupying incompatible positions (small $\mathbf{x}^{\perp}$). These points are then replaced by a single atom at their average position $\mathbf{x}^{\parallel}$. Equations (4) and (5) define, given two (or more) interpenetrating lattices in physical space, an ideal, best fit, minimum strain lattice as the set of points $\mathbf{x}^{\parallel}$. Since strain is a physical consideration, this endows the formalism with a physical basis in spite of its geometrical formulation. While $\mathbf{E}^{\parallel}$ contains lattice points, $\mathbf{E}^{\perp}$ contains displacements and is therefore associated with the displacement space called *b* space by Bollmann.[14]

By adopting the average position $\mathbf{x}^{\parallel}$, atoms in the interface act as a strain buffer between the crystals on each side of the interface[12] that minimizes the elastic energy. The $\mathbf{x}^{\perp}$ component is thus a measure of the local strain at $\mathbf{x}^{\parallel}$ representing the frustration between two nearly coincident positions.

It is natural to assume that the interfacial energy should be lower in regions of small local strain. In particular, when $\mathbf{x}^{\perp}=0$, the point $\mathbf{x}^{(1)}=\mathbf{x}^{(2)}$ is a coincidence with zero local strain. Note that since a rational relationship is assumed between $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$, an infinite number of hyperlattice points $\{\mathbf{x}^c\}$ intersect $\mathbf{E}^{\parallel}$ with zero local strain defining the CSL. Since every interfacial point $\mathbf{x}^{\parallel}$ has an associated strain $\mathbf{x}^{\perp}$, the configuration of points in $\mathbf{E}^{\perp}$ is a reduced representation of the local strain in $\mathbf{E}^{\parallel}$. In principle, for incommensurate interfaces (or quasicrystals) the distance $|\mathbf{x}^{(1)}-\mathbf{x}^{(2)}|$ becomes arbitrarily small (but not zero except at the origin) and $\mathbf{E}^{\perp}$ becomes densely filled. However, assuming a rational orientation, a discrete structure appears in $\mathbf{E}^{\perp}$ which can be used to characterize the interface and calculate its diffraction properties.

From the projectors $\mathbf{\Pi}$ and $\mathbf{\Pi}^{\perp}$ it is easy to show that the reflection

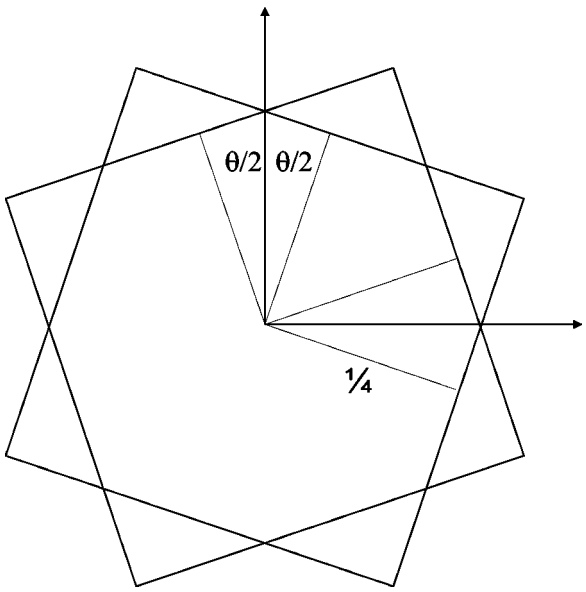

FIG. 2. Projection window of cubic ⟨001⟩ twist GB's defined by the intersection of the basal planes of two cubes rotated by $\pm\theta/2$. The edge of the cubes is half the minimum interatomic distance. The rotation axis is normal to the page.

$$\mathbf{R}=\mathbf{R}^{-1}=\frac{1}{\sqrt{2}}\begin{pmatrix}\mathbf{I} & \mathbf{I}\\ \mathbf{I} & -\mathbf{I}\end{pmatrix} \tag{6}$$

relates the coordinate systems of $(\mathbf{V}_1,\mathbf{V}_2)$ and $(\mathbf{E}^{\parallel},\mathbf{E}^{\perp})$ so that

$$\mathbf{R}(\mathbf{x}^{(1)},\mathbf{x}^{(2)})=(\mathbf{x}^{\parallel},\mathbf{x}^{\perp}). \tag{7}$$

C. Window

The intersection of the strip with $\mathbf{E}^{\perp}$ defines a bounded region called projection window (Fig. 1). Only those hyperpoints whose $\mathbf{x}^{\perp}$ component falls within this window are eligible for projection into physical space. As an example, in the case of rotation-related lattices there are no displacements parallel to the rotation axis $\boldsymbol{\rho}$ and the window is a 2D plane segment perpendicular to $\boldsymbol{\rho}$. If the strip is chosen so that $\mathbf{x}^{(1)}-\mathbf{x}^{(2)}$ is less than half the interatomic distance, then the strip is a hypercylinder and the window a sphere of radius $d/4$, with d being the minimum interatomic spacing. Although this window produces the normal set of O points predicted by Bollmann[14] for low-angle fcc ⟨001⟩ twist GB's, it does not account for the extra O points found experimentally.[10] These results are reproduced by a different window defined as the intersection of the plane normal to $\boldsymbol{\rho}$ and two solid cubes rotated by $\pm\theta/2$ around $\boldsymbol{\rho}$ as shown in Fig. 2. This window accepts hyperpoints $(\mathbf{x}^{(1)},\mathbf{x}^{(2)})$ with the property that $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ lie in the intersection of their respective Wigner-Seitz cells.[18] Such points are referred to as quasicoincidences and lead to structures that are stable upon static relaxation.[12]

Note the price paid in loss of hyperlattice symmetry is compensated by the physical interpretation that can now be given to the lattice points in $\mathbf{E}^{\parallel}$ and $\mathbf{E}^{\perp}$ through Eqs. (4) and (5). Moreover, since the symmetry of the hyperlattice changes with the orientation between parent crystals, it can be related to orientational variants.

V. INTERFACES AND QUASICRYSTALS AS COMPETING LATTICES

The interface is a region in space where two lattices, each representing the ground state of a crystal, are forced to coexist. In this scenario, the modified strip-projection method can be seen as a referee that determines, using a minimum strain criterion, the final structure in the region of conflict.

Since the method describes equally well interfaces and quasicrystals, it is only natural to extend this interpretation to quasicrystals and consider them as ''best fit'' structures resulting from 3D lattices competing for space. If such lattices were found (possibly from the crystalline phases surrounding the quasicrystal in the phase diagram), the method could yield the ''best fit'' atomic structure (a decorated tiling) of a quasicrystal.

The average lattice given by Eq. (4) should be a plausible low-energy configuration for metallic close-packed structures where the interatomic potential is mostly isotropic,[12] which is a possible reason why quasicrystals have only been found in metal alloys. The same interpretation should still hold for covalent systems, although the formalism would have to include a way of accounting for bonding anisotropies.

Under ideal conditions (such as a perfectly isotropic potential) it is sensible to assume that the ground state of an interface minimizes local strain. By comparing the diffraction patterns calculated from minimum strain interfaces with actual measurements, the pertinence of such ''perfect'' structures could be assessed and defects in real interfaces could be identified as it is commonly done for crystals. The diffraction equations for perfect interfaces derived from the distribution of points in $\mathbf{E}^{\perp}$ shall be presented in a forthcoming publication.

Interfacial manifold

When all the points within the strip are projected onto $\mathbf{E}^{\parallel}$, the result is a 3D structure, yet in contrast with quasicrystals, interfaces are mostly two-dimensional systems. This can be understood as follows: when the energy density in the region occupied by the projected points is larger than that of the adjacent crystals, the region minimizes its volume by collapsing into a 2D surface. When the opposite is true, all points in the strip are projected and a new 3D phase (such as a quasicrystal) nucleates between the two crystals.

The set of hyperpoints $\{(\mathbf{x}^{\parallel},\mathbf{x}^{\perp})\}$ that project onto a planar interface define a 2D manifold within the strip in $\mathbf{R}^6$. In this scenario, the problem of calculating the atomic structure of an interface, now including the orientation of the boundary plane, is replaced by the geometrical problem of finding the 2D manifold that minimizes the energy of the system. For those systems whose interfacial energy is minimized by reducing local strain, a manifold that goes through hyperpoints with minimum $\mathbf{x}^{\perp}$ component (closest to $\mathbf{E}^{\parallel}$) should yield an accurate interfacial structure.

VI. CHARACTERIZATION OF INTERFACES

A. Symmetry variants

Any relative rigid body translation $\mathbf{b}=(b_1,b_2,b_3)$ between $\mathbf{\Lambda}_1$ and $\mathbf{\Lambda}_2$ is taken into account from the median lattice by displacing $\mathbf{\Lambda}_1$ by $\mathbf{b}/2$ and $\mathbf{\Lambda}_2$ by $-\mathbf{b}/2$. This is equivalent to displacing the whole hyperlattice by the 6D vector $\hat{\mathbf{b}}=(b_1,b_2,b_3,-b_1,-b_2,-b_3)/2$. It is easy to show using Eqs. (4) and (5) that $\mathbf{b}^{\parallel}=\mathbf{\Pi}(\hat{\mathbf{b}})=\mathbf{0}$ and $\mathbf{b}^{\perp}=\mathbf{\Pi}^{\perp}(\hat{\mathbf{b}})=\mathbf{b}$. Therefore, all crystal displacements are completely contained in $\mathbf{E}^{\perp}$. As a result, Eq. (4) does not change upon relative lattice translations but Eq. (5) becomes

$$\mathbf{x}^{\perp}=\mathbf{\Pi}^{\perp}(\mathbf{x}+\hat{\mathbf{b}})=\frac{1}{2}[(\mathbf{x}^{(1)}-\mathbf{x}^{(2)})]+\mathbf{b}. \tag{8}$$

This implies that a relative crystal translation has the effect of displacing the strip along $\mathbf{E}^{\perp}$, leaving the hyperlattice undisturbed, thus decoupling the translational and orientational degrees of freedom.

One must bear in mind that a strip displacement may cause a different set of hyperpoints $(\mathbf{x}^{(1)},\mathbf{x}^{(2)})$ to be projected onto $\mathbf{E}^{\parallel}$. Such displacements may change the symmetry of the real space structure,[9] leading to structural variations known in the interfaces field as translational states[19] or translational variants.[2] However, a displacement of the strip does not change the symmetry class or local isomorphism[9] of the structure which depends solely on the relative orientation (and symmetry) of the parent crystals. This significantly simplifies the characterization task using dichromatic patterns whose symmetry changes unpredictably with relative crystal displacements.[3]

In this framework, an interface can be fully characterized (prior to the introduction of a boundary surface) by the symmetry of the hyperlattice and the position of the strip along $\mathbf{E}^{\perp}$. Each orientational variant, described by the symmetry of the hyperlattice, corresponds to a local isomorphism, and each local isomorphism has a number of symmetry-inequivalent translational variants described by the position of the strip. In the following sections we shall see that the number of orientational and translational variants for rotational interfaces is (effectively) finite.

B. Phason dislocations

In order to preserve the smallest $\mathbf{x}^{\perp}$ components, a shift of the strip is normally accompanied by a change in the shape of the projection manifold. If the strip (or manifold) is displaced by a vector $\mathbf{b}^{\perp}$ (Fig. 3) so that it intersects another hyperpoint, the real space structure is the same as before, with an inconsequential shift of origin ($\mathbf{b}^{\parallel}$ in Fig. 3) in parallel space. The same origin shift is obtained by displacing the strip by the vector $\mathbf{b}=3\mathbf{x}^{(1)}+2\mathbf{x}^{(2)}$ which projects onto the DSCL vector $\mathbf{b}^{\parallel}=3\Pi(\mathbf{x}^{(1)})+2\Pi(\mathbf{x}^{(2)})$. Since the full hyperlattice projects onto the DSCL [Eq. (4)], displacements through hyperlattice vectors always preserve the translational state of the interface; therefore, relative translations need only be specified modulo a DSCL vector. In what follows, we shall refer to non-DSCL displacements as phasons.

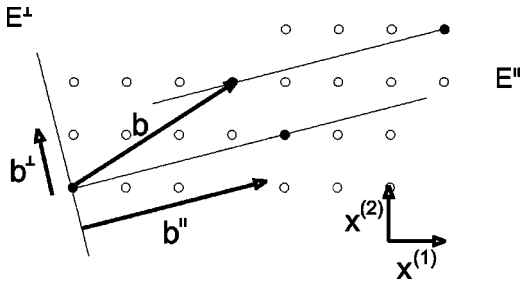

FIG. 3. Displacing the projection manifold by $\mathbf{b}^{\perp}$ so that it intersects another hyperpoint is equivalent to shifting the hyperlattice by one of its vectors. This shifts the real space structure by the (DSCL) vector $\mathbf{b}^{\parallel}=3\Pi(\mathbf{x}^{(1)})+2\Pi(\mathbf{x}^{(2)})$, leaving it otherwise unaltered.

Although it is normally assumed that extrinsic dislocations dissociate into dislocations with Burgers vectors belonging to the DSCL, this is not necessarily the case. When a crystal dislocation enters a GB, it becomes an extrinsic GB dislocation and introduces a local displacement manifested as a step in the strip and manifold. If the resulting increase in elastic energy is too large, the dislocation may dissociate into smaller components that lead to lower-energy translational states and a smoothing of the strip. It is possible that translational states arrived at by phasons manifested as partial DSCL dislocations[12] are energetically preferred. Since IGB's already contain a mixture of translational states, there is no fundamental state to be preserved by DSCL dislocations.

VII. HYPERLATTICE OF ROTATION-RELATED CRYSTALS

A practical application of the formalism will be exemplified here using the well-known case of rotation interfaces. Consider two lattices such that $\hat{\mathbf{L}}_2=\mathbf{M}^2\hat{\mathbf{L}}_1$ [see Eq. (1)]. The hyperlattice is defined in the 6D median lattice by the hyperstructure matrix

$$\hat{\mathbf{L}}^{(6)}=\sqrt{2}\begin{pmatrix}\mathbf{M}^{-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{M}\end{pmatrix}\begin{pmatrix}\hat{\mathbf{L}}_1 & \mathbf{0}\\ \mathbf{0} & \hat{\mathbf{L}}_2\end{pmatrix}. \tag{9}$$

Projection onto $\mathbf{E}^{\parallel}$ and $\mathbf{E}^{\perp}$ generates two lattices with structure matrices $\mathbf{L}^{\parallel}$ and $\mathbf{L}^{\perp}$ given by

$$\hat{\mathbf{L}}^{\parallel}_m=\frac{1}{2}(\mathbf{M}^{-1}\hat{\mathbf{L}}_1+\mathbf{M}\hat{\mathbf{L}}_2), \tag{10}$$

$$\hat{\mathbf{L}}^{\perp}_m=\frac{1}{2}(\mathbf{M}^{-1}\hat{\mathbf{L}}_1-\mathbf{M}\hat{\mathbf{L}}_2). \tag{11}$$

Note that $\hat{\mathbf{L}}^{\perp}$ is basically the Frank-Bilby equation giving the displacement field at the interface which confirms the consistency between the formalism and known theory. The columns of $\hat{\mathbf{L}}^{\parallel}_m$ and $\hat{\mathbf{L}}^{\perp}_m$ are the basis vectors of two lattices in the corresponding spaces.

In view of the minimum $\mathbf{x}^{\perp}$ requirement, the manifold has a stepped shape which causes the appearance of dislocation networks in the real space structure. This means that all in-

terfaces are composed of atomic domains limited by dislocations. If the dislocations belong to the DSCL, then all domains belong to the same translational state. Otherwise the symmetry of adjacent domains is different.[12] As a result, $\hat{\mathbf{L}}_m^{\parallel}$ describes only the structure of the central, dislocation-free, domain near the origin.

In particular, for identical crystal lattices, $\mathbf{L}_1=\mathbf{L}_2=\mathbf{L}_m^{(3)}$ and $\mathbf{M}^2=\mathbf{R}_\theta$ (a rotation through θ around $\hat{\rho}=\langle hkl\rangle$). Then $\mathbf{M}=\mathbf{R}_{\theta/2}$ and

$$\mathbf{L}_m^{\parallel}=\frac{1}{2}(\mathbf{R}_{-\theta/2}+\mathbf{R}_{+\theta/2})\mathbf{L}_m^{(3)}, \tag{12}$$

$$\mathbf{L}_m^{\perp}=\frac{1}{2}(\mathbf{R}_{-\theta/2}-\mathbf{R}_{+\theta/2})\mathbf{L}_m^{(3)}, \tag{13}$$

where the operators

$$\mathbf{R}^{\parallel}=\frac{1}{2}(\mathbf{R}_{-\theta/2}+\mathbf{R}_{+\theta/2}), \tag{14}$$

$$\mathbf{R}^{\perp}=\frac{1}{2}(\mathbf{R}_{-\theta/2}-\mathbf{R}_{+\theta/2}) \tag{15}$$

are the symmetric and antisymmetric components of $\mathbf{R}_{-\theta/2}=\mathbf{R}^{\parallel}+\mathbf{R}^{\perp}$. The CSL is given by the null space of $\mathbf{R}^{\perp}$, and in median lattice coordinates, the O lattice is given by $(2\mathbf{R}^{\perp})^{-1}$.

VIII. ROTATION-RELATED BOUNDARIES IN THE CUBIC SYSTEM

A. Generalized Ranganathan's expression

By considering all GB's as periodic, Ranganathan's equation[20] can be applied to all interfaces in the cubic system. Accordingly, given two cubic lattices related by a rotation through θ around $\langle hkl\rangle$ we have

$$\tan\frac{\theta}{2}=\sqrt{N}\,\frac{p}{q}, \tag{16}$$

with p and q being arbitrary coprime positive integers and $N=h^2+k^2+l^2$. The index number Σ is given by (divided by 2 until odd)

$$\Sigma=q^2+Np^2. \tag{17}$$

There are significant advantages in rewriting Eq. (16) in the form

$$\tan\frac{\theta}{2}=\sqrt{N}\,\frac{1}{x+\delta}=\sqrt{N}\,\frac{1}{\xi}, \tag{18}$$

where $\xi=\sqrt{N}\cot\theta/2=x+\delta$ with x and δ being the integer and fractional parts of $\sqrt{N}\cot\theta/2$. If the closest integer function is used to evaluate x, then δ lies in the interval $[-0.5,0.5)$; if the integer function is used instead, δ lies within $[0,1)$.

Equation (18) is a generalization of Ranganathan's equation to irrational orientations since now δ can acquire irrational values. This means that Eq. (18) also describes, if one so wishes, nonperiodic interfaces taken in a strict mathematical sense (see Fig. 4). If δ is a rational number, it reduces to Eq. (16). Its most significant advantage, however, lies in that unlike p and q, x and δ are given in terms of the experimental observables θ and N and are thus linked to the geometry of the interface.[12] In terms of x and δ, the index number becomes

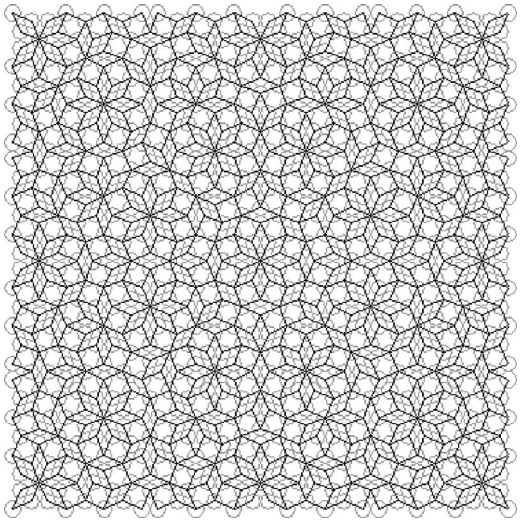

FIG. 4. Cubic twist $\langle 001\rangle$ interfacial plane with quasicrystalline octagonal symmetry obtained with $\theta=45$, $x=3$, $\delta=\sqrt{2}-1$. Gray circles indicate atomic positions.

$$\Sigma=p^2[(x+\delta)^2+N]. \tag{19}$$

DGB's occur when[12] $\delta=0$ ($p=1$, $\xi=x$), so that Eqs. (18) and (19) become

$$\tan\frac{\theta_x}{2}=\sqrt{N}\,\frac{1}{x}, \tag{20}$$

$$\Sigma_x=x^2+N. \tag{21}$$

δ is referred to as the deviation parameter since it is a measure of the angular separation between a general IGB with rotation angle θ and its closest DGB at the singular angle θ_x.

Note that for IGB's the integer p takes part in the expression of Σ [Eq. (19)]. Since p cannot be experimentally determined, Σ is ill defined for these boundaries. On the other hand, DGB's have a well-defined Σ given in terms of the measurable angle θ_x [Eq. (21)]. This leads to an alternative definition of DGB's as those with a well-defined index number Σ_x.

Ranganathan's expression for epitaxial interfaces

The generalized Ranganathan's expression can also be used for epitaxial interfaces between two lattices of different lattice parameter. Let $\mathbf{L}_1,\mathbf{L}_2$ be two lattices such that $\mathbf{L}_2=\alpha\mathbf{L}_1$, with $\alpha=p/q$, p,q being two coprime integers such that $p<q$. If, in analogy with Eq. (18), we define

$$\alpha = \frac{p}{q} = \frac{1}{x+\delta}, \tag{22}$$

where x is the integer part of q/p and $\delta = \alpha - x$, then we can write

$$\mathbf{L}_2 = \frac{1}{(x+\delta)}\mathbf{L}_1. \tag{23}$$

In analogy with the case of rotation related GB's, we can now define delimiting GB's as those for which $\delta = 0$, i.e., $p=1$, $q=x$, and $\mathbf{L}_1 = \mathbf{x}\ \mathbf{L}_2$. Hence delimiting expitaxial boundaries occur when $\mathbf{L}_1$ is a sublattice of $\mathbf{L}_2$. Since for expansion-related interfaces $\mathbf{M}$ [see Eq. (1)] is given by

$$\mathbf{M} = \sqrt{p/q}\mathbf{I} = \frac{1}{\sqrt{x+\delta}}\mathbf{I}, \tag{24}$$

the O and CSL lattices are given (in the median lattice) by

$$\mathbf{O} = \frac{\sqrt{pq}}{p-q}\mathbf{L}_1 = \frac{\sqrt{x+\delta}}{1-(x+\delta)}\mathbf{L}_1 \tag{25}$$

and

$$\mathbf{C} = \sqrt{pq}\mathbf{L}_1 = p\sqrt{x+\delta}\mathbf{L}_1. \tag{26}$$

Note the O lattice diverges for $x=1$, $\delta=0$, which means that misfit dislocations become infinitely spaced when $\mathbf{L}_1 = \mathbf{L}_2$. Also note that $\mathbf{C}$ is again ill defined for nondelimiting GB's since there is no experimental access to p.

B. Class of small-angle boundaries

If θ is small, $x+\delta$ is a large number and its fractional part δ can be neglected. Hence, small-angle boundaries are effectively delimiting boundaries, and like any other DGB, they must contain only primary dislocations, as it is indeed observed.[12] This makes it clear why small-angle boundaries are in a class of their own: they are so close together ($x \gg \delta$) that no intervening boundaries are found around them, and it is no longer justifiable to call them singular. As a result, although the number of delimiting boundaries is actually infinite, only a finite number of them are singular.

C. Crystallography of ⟨001⟩ twist boundaries

A boundary plane (a 6D manifold) must now be introduced. For simplicity, we shall consider here the relatively simple case of cubic ⟨001⟩ twist boundaries with the purpose not to obtain a full crystallographic characterization of the system at this point, but rather as an illustration of the principles involved in the task. In this section the P lattice will be defined for this system and its relation to other lattices explored. Also, existing theory shall be discussed and restated in the HD framework using results from the GCSN model.[12]

The interface of ⟨001⟩ twist GB's consists of a single buffer plane,[12] although it must be noted that this is not the general case; the interface of low-angle ⟨011⟩ twist DGB's, for instance, can be stepped.[11] Predicting nonplanar boundary surfaces is possible in this approach because it gives the best fit regions in a volume containing interpenetrated, as opposed to just juxtaposed, crystal lattices.

The O lattice provides the primary dislocation content of DGB's and for rotation-related boundaries it is given in median lattice coordinates by the transformation

$$\mathbf{O}_\xi = (2\mathbf{R}^\perp)^{-1} = \frac{\sqrt{\xi^2+N}}{2\sqrt{N}}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{27}$$

with $N=1$ for ⟨001⟩ twist GB's. The O lattice $\mathbf{O}_x$ of delimiting GB's is obtained by substituting $\delta=0$, $N=1$ in Eq. (27):

$$\mathbf{O}_x = \frac{\sqrt{x^2+1}}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{28}$$

Subindexes x and ξ are used to distinguish between delimiting and intervening lattices.

D. Delimiting boundaries

The boundary plane of DGB's ($\delta=0$) is composed of atomic domains delimited by a network of primary dislocations (see Fig. 5) as can be verified by applying the Frank-Bilby equation to $\mathbf{O}_x$. Since primary dislocations have crystalline Burgers vectors belonging to the DSCL, all domains belong to the same translational state and differ only in size (the length of the $\mathbf{O}_x$ vectors), which is an increasing function of x. The structure of this unique domain type is the same as that of the trivial $x=1$, $\delta=0$, $\Sigma=1$ boundary (an (001) crystal plane).

Although all delimiting domains have the same structure, they differ in the relative displacement of their points with respect to the O point at their center. Domains labeled A, B, and C, in Fig. 5 with O points colored black, gray, and white are, respectively, shifted by the vectors with coordinates $\{0,0\}$, $\frac{1}{2}\{1,1\}$, and $\frac{1}{2}\{0,1\}$, given in terms of the base vectors of the median lattice. This introduces a partition of the O lattice into three sublattices (A, B, C) according to the type of domain at the center of which they lie. As we shall see, the domains of intervening boundaries and the points of the P lattice can be equivalently partitioned.

The CSL $\mathbf{C}$ can have two orientations depending on the parity of x (Ref. 12): the parallel orientation (x even) in which $\mathbf{C} \| \mathbf{O}$ and the inclined orientation (x odd) where $\mathbf{C}$ and $\mathbf{O}$ are rotated by $\pi/4$. The inclined orientation has O points of types A and B, while the parallel orientation also has type-C O points. The CSL always coincides with the sublattice of type-A O points (Fig. 5).

Since $\mathbf{C}$ is a sublattice of $\mathbf{O}$, there exists a transformation $\mathbf{K}$ such that $\mathbf{C} = \mathbf{KO}$. For the ⟨001⟩ twist case in the parallel orientation $\mathbf{K} = 2p\mathbf{R}_{\pi/2}$ while for the inclined orientation $\mathbf{K} = p\mathbf{R}_{\pi/4}$. Since Σ is only well defined for DGB's ($p=1$), we shall only consider the CSL of delimiting boundaries $\mathbf{C}_x$ which can be written for any orientation as

$$\mathbf{C}_x = \mathbf{KO}_x = \mathbf{F}^\nu \mathbf{O}_x, \tag{29}$$

where $\mathbf{F} = \sqrt{2}\mathbf{R}_{\pi/4}$, $\nu = 1 + (x^2+1) \bmod 2$, with mod being the modulo function and $\nu = 1,2$ for x odd, even.

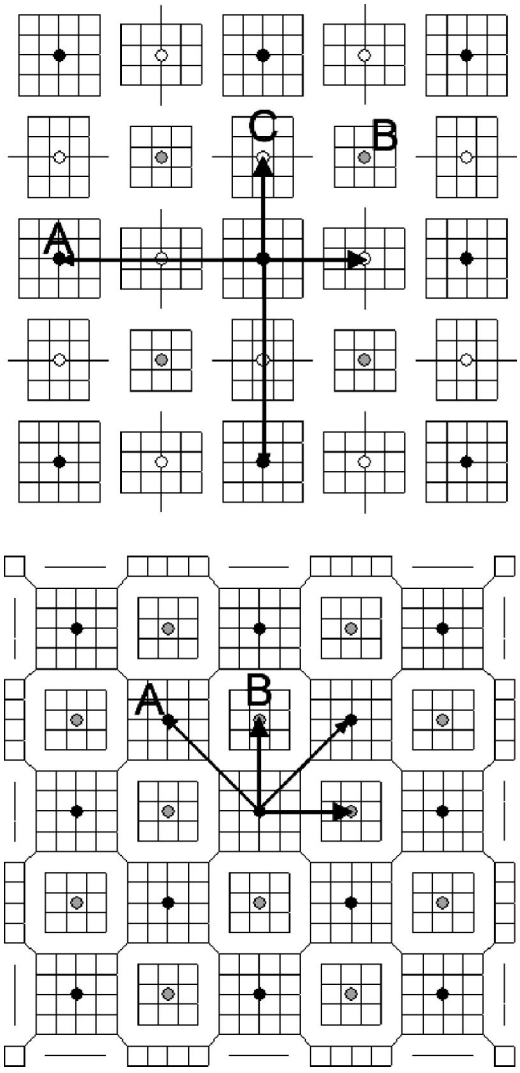

FIG. 5. Wire figure (lines joining nearest neighbors) of delimiting simple cubic ⟨001⟩ twist boundaries for parallel (top) and inclined (bottom) relative orientations of the O and CSL lattices. O lattice: short thick arrows. CSL: long narrow arrows. Note that the periodicity of domain types is the same as that of the CSL.

Following Grimmer *et al.*,[21] the DSCL is given by $\mathbf{D}=(\mathbf{C}^T)^{-1}$ and for delimiting boundaries it can be obtained from Eq. (29):

$$\mathbf{D}_x=\frac{1}{2^\nu}\frac{4}{1+\xi^2}\mathbf{F}^\nu\mathbf{O}_x. \tag{30}$$

E. Intervening boundaries

The O lattice does not describe the dislocation content of IGB's. According to Bollmann[14] the structure (i.e., the translational variant) of boundaries near DGB's (small δ) must be preserved. To achieve this, he postulates that these boundaries should possess a network of dislocations with Burgers vectors belonging to the DSCL ($\mathbf{D}_x$) of the nearby singular orientation θ_x. The secondary O lattice **S** is then defined as the dual of the secondary dislocation network.

One problem of this reasoning is that no unambiguous definition ($\delta=0$) of DGB's existed until recently, and without it, it was not clear when to use the primary or secondary O lattices to describe the dislocation content of an interface. The usual small-Σ criterion is not enough since, as we have seen, it leads to inconsistencies. For instance, $\Sigma 29$ has a smaller period than $\Sigma 41$; however, the former is an IGB ($x=2$, $\delta=1/3$) containing nonprimary dislocations while $\Sigma 41$ is a DGB ($x=9$, $\delta=0$) with a purely primary dislocation content. Another problem of the argument is that it says nothing about the structure of GB's far from special orientations.

In spite of this, **S** is still fundamental to the description of interfaces since it provides the distribution of sites in the interface that belong to the same translational state. Following Bollmann, to calculate **S** we must first calculate the DSCL of a DGB at θ_x. The secondary O lattice at $\theta_x+\Delta\theta$ is then given by $\mathbf{S}_\xi=\mathbf{O}_\beta\mathbf{D}_x$ [see Eqs. (27) and (30)], with β being the value of ξ resulting from substituting θ by $\Delta\theta=\theta-\theta_x$ in Eq. (18). Thus, in the median lattice, $\mathbf{S}_\xi$ is given by

$$\mathbf{S}_\xi=\frac{1}{2\delta}\sqrt{x^2+1}\sqrt{\xi^2+1}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\mathbf{D}_x \tag{31}$$

or, in terms of $\mathbf{O}_\xi$,

$$\mathbf{S}_\xi=\mathbf{F}^{2-\nu}(\delta^{-1}\mathbf{O}_\xi). \tag{32}$$

Similar expressions exist for the other rotation axes in the cubic system, i.e., a function of **K**, in this case $\mathbf{F}^{2-\nu}$, applied to the scaled O lattice $\delta^{-1}\mathbf{O}_\xi$. Since **K** is a relatively simple function to calculate,[21] this method represents a simplified way to calculate **S**.

Intervening interfaces also contain atomic domains defined by dislocation networks,[12] but here the Burgers vectors of these dislocations are not DSCL vectors but phasons, so that adjacent domains belong to different translational states (see Fig. 6).

The structure of intervening interfaces in the angular range defined by $\xi\in(x-1/2,x+1/2)$ is the same except for domain size (dislocation spacing), which increases as $\xi\to x$ ($\delta\to 0$) in accordance with experimental observations.[22,23] At the singular angle $\theta=\theta_x$ the domain containing the origin becomes infinitely large and the GB becomes delimiting.

Intervening domains have the structure of some of the translational states of the delimiting boundary Σ_x at $\xi=x$ ($\delta=0$). These states are obtained by projecting the hyperlattice of Σ_x with a strip shifted by a vector within the Wigner-Seitz cell of $\mathbf{D}_x$ (see Fig. 7). Although the number of vectors (phasons) in this cell is nondenumerable, the number of different translational states is finite. This occurs as a direct consequence of the discrete nature of the hyperlattice: while displacing the strip, the projected structure remains unchanged until eventually one or more hyperpoints (per unit cell) enter and/or leave the strip. As an example, Fig. 7 shows the translational states of $\Sigma_5(x=3,\delta=0)$, as a function of the strip displacement.

The structure of any IGB at $\theta_{x+\delta}$ is thus determined by the structure of the closest delimiting boundary at θ_x (δ

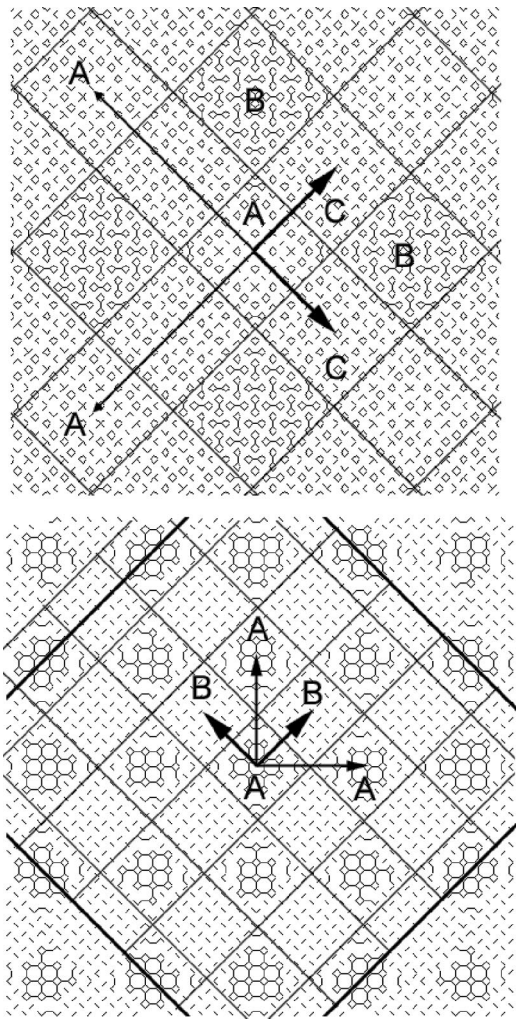

FIG. 6. Wire figure of intervening interfaces corresponding to (top) parallel state ($\Sigma=21389$, $x=4$, $\delta=2/35$) showing domain types A, B, C and (bottom) inclined state ($\Sigma=4369$, $x=3$, $\delta=3/20$) with domains A and B. The secondary O-lattice vectors, marked with long thin arrows, join domains of same type (A-A) while the P lattice (short thick arrows) joins domains of different types. The CSL unit cell of $\Sigma=4369$ is drawn, but that of $\Sigma=21\,389$ is too large to be shown. The properties of intervening GB's are determined by the domain periodicity and not by that of the CSL.

$=0$) (Ref. 12) as a mixture of its translational states. This partitions the angular range into regions limited by ($x-1/2$, $x+1/2$). Each region representing an orientational variant of the $\langle 001\rangle$ twist system. Since for large x (small θ) all GB's become delimiting, the number of orientational variants is finite, and since the number of translational states per orientational variant is also finite, it becomes possible to characterize the symmetry of any GB.

The P lattice is defined as the set of points that join domains of different symmetry (Fig. 6) or, more precisely, as the dual lattice of the phason dislocation network, in direct analogy with the O lattice which is the dual of the primary dislocation network. In terms of the conventional O lattice, the P lattice is given by

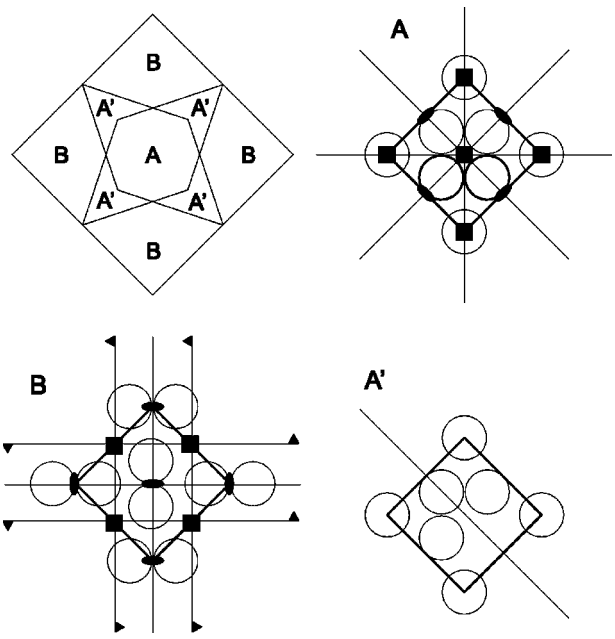

FIG. 7. Top left: Wigner-Seitz cell of the DSCL of $\Sigma 5$ ($x=3,\delta=0$) cubic twist $\langle 001\rangle$ interface. The regions marked A, A′, B indicate the translational states arrived at by the corresponding displacement vector. The accompanying figures show the $\Sigma 5$ unit cell decorated with circles at lattice points to aid in the visualization of structural units and symmetry elements present in each state. Note states A and A′ differ only by the removal of one atom. Since the good fit criterion is determined by the strip, a slight variation of the window contour could leave this atom in place. The determination of atomic structure at this level of detail requires additional computer relaxation allowing atomic diffusion. Note domain types A and B contain the same symmetry elements of Bristowe and Crocker's types 2 and CSL (Ref. 19).

$$\mathbf{P}_\xi=\mathbf{F}^{2(1-\nu)}(\delta^{-1}\mathbf{O}_\xi). \tag{33}$$

With the aid of Eqs. (32) and (33), $\mathbf{P}_\xi$ can be expressed in terms of the secondary O lattice (Fig. 6) which joins domains of the same type:

$$\mathbf{S}_\xi=\mathbf{F}^\nu\mathbf{P}_\xi. \tag{34}$$

Figure 6 shows that intervening GB's also have up to three different domain types distinguished by their symmetry, each corresponding to a translational state of Σ_x. Just as for delimiting boundaries, the inclined orientation contains two types of domains A and B, while the parallel orientation has an additional type C. A detailed account of the translational states present in each orientational variant shall be presented elsewhere.

Just as the size of the smallest O-lattice vectors gives the spacing between primary dislocations, the phason dislocation spacing s is given by the magnitude of the smallest P-lattice vectors (Fig. 6), which can be expressed in terms of the angles as

$$s=\frac{1}{2\nu}\frac{1}{\cos\frac{\theta}{2}-x\sin\frac{\theta}{2}}=\frac{1}{2\nu}\frac{\sin\frac{\theta_x}{2}}{\sin\frac{\Delta\theta}{2}}, \tag{35}$$

where $\Delta\theta=\theta-\theta_x$. This equation is in agreement with experimental observations[12,22,23] and constitutes strong support for the formalism. Phason dislocations are in fact partial secondary dislocations, and the difference in the structure of adjacent domains corresponds to the stacking fault associated with this type of dislocation. The displacements associated with the secondary O-lattice vectors, on the other hand, belong to the DSC lattice and preserve symmetry so that it joins domains with equal symmetry as shown in Fig. 6.

F. General considerations

Figures 5 and 6 show that delimiting and intervening boundaries are topologically identical, the difference being the symmetry of the domains and the Burgers vector of the dislocation networks that define them. Delimiting domains have all the same symmetry and dislocation networks given by the dual of the O lattice. Intervening domains, on the other hand, have different symmetries determined by the translational states of the associated delimiting boundary and are the dual of the P lattice. This equivalence is mathematically expressed by the similarity of Eqs. (29) and (34).

The lattice pairs $(\mathbf{O}_x,\mathbf{C}_x)$ and $(\mathbf{P}_\xi,\mathbf{S}_\xi)$ play symmetrical roles in the description of DGB's and IGB's. These lattices are sufficient to completely characterize all interfaces except for the structural units within each domain determined by the translational states of the closest delimiting GB. This means that the structure and hence the properties of IGB's are determined by the periodicity of the domain types ($\mathbf{C}_x$ or $\mathbf{S}_\xi$) and not by the strict period Σ which is ill defined and pathologically discontinuous.

All that remains to do for a full crystallographic characterization of the system is to describe the symmetry properties and the structural units of each domain type. The number of translational states in each orientational variant increases with x; however, only the ones with highest symmetry are chosen by the cut-projection method to define the interface. The detailed calculation of the translational states present in each local isomorphism and which of them are selected to form the interface shall be deferred to a forthcoming publication.

IX. CONCLUSIONS

It has been shown that in a higher-dimensional approach, quasicrystals and interfaces are formally equivalent. This is an important result since describing under the same formal context two apparently unrelated physical systems always enhances our understanding of nature as a whole. In this framework, interfaces and quasicrystals are interpreted as a region in space where the atoms of interpenetrated crystal lattices compete for space, with a modified strip-projection method deciding the final atomic positions. Based on this paradigm, a method derived from the strip-projection formalism has been introduced. The method produces ideal (minimum local strain) structures. Since minimum strain is a physical consideration, this gives the method a physical basis in spite of its geometrical formulation.

Ideal interfaces are suggested to play an analogous role in grain boundaries to that played by the perfect crystal and quasicrystal concepts in the study of crystals and quasiperiodic structures, thus constituting an important step towards the formulation of a general crystallographic theory of interfaces. This hypothesis is supported by the ability of ideal interfaces to quantitatively account for some experimental observations on fcc twist boundaries. Also, when the hyperlattice is projected in perpendicular space, the Frank-Bilby equation is rederived. The fact that such a general result can be obtained from this approach constitutes further evidence in favor its ability to describe interfacial-related phenomena.

Some advantages of the modified strip-projection method are the following: (a) It has given a new meaning to perpendicular space by associating it with Bollmann's b space. (b) Since a geometrical link exists between the 6D hyperlattice and the 3D competing lattices, the method produces, in contrast with other approaches, already decorated tilings. (c) It suggests that quasicrystals can grow at the interface of properly oriented crystals, a prediction that can lead to the discovery of new quasicrystalline phases in systems so far unexplored.

Other advantages of the method are the following: The effect of dislocations impinging on grain boundaries can be described in terms of strip displacements by the Burgers vector of the dislocation. This is useful in describing the interaction between crystal dislocations and grain boundaries, related to mechanical properties of policrystals.

It has introduced a new classification of interfaces in well-defined equivalence classes that include orientational and translational degrees of freedom. This classification is based on the symmetry of the hyperlattice and the position and shape of the strip and is consistent with previous structural units and symmetry approaches. Each orientational variant, described by the symmetry of the hyperlattice, corresponds to a local isomorphism, and each local isomorphism has a number of symmetry-inequivalent translational variants. The number of both orientational and translational variants is finite, and it is hoped that such classes can be later associated with the physical properties of interfaces.

It has been shown that the structure and hence the properties of GB's are determined by the periodicity of the isosymmetrical regions (domain types) and not by the strict boundary period Σ which is ill defined (except for DGB's). For delimiting boundaries this periodicity is given by the CSL while for IGB's it is given by the secondary O lattice.

The phason or P lattice has been introduced to describe the dislocation content of IGB's. The P and O lattices play symmetrical roles in accounting for the dislocation content of intervening and delimiting boundaries, respectively.

ACKNOWLEDGMENT

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