arXiv:cond-mat/0211687v1 [cond-mat.mtrl-sci] 29 Nov 2002

PHASONS AND THE PLASTIC DEFORMATION OF QUASICRYSTALS

MAURICE KLEMAN

Laboratoire de Minéralogie-Cristallographie (UMR CNRS 7590)
Universités de Paris-VI & de Paris-VII, case 115, 4 place Jussieu,
75252 Paris cédex 05

ABSTRACT

The plastic deformation of quasicrystals (QC) is ruled by two types of singularities of the QC order, singularities of the 'phonon' strain field, and singularities of the 'phason' strain field. In the framework of the general topological theory of defects, in which the QC is defined as an irrational subset of a crystal of higher dimension, both types of defects appear as distinct components of the same entity, called a *disvection*[2]. Each of them can also be given a description in terms of more classical concepts, within a detailed analysis of the Volterra process: it can be shown that (a)- the phonon singularity breaks some symmetry of translation, represented by its Burgers vector $\mathbf{b}_{||}$ projected from a high dimensional crystalline lattice onto the physical space; it is therefore akin to a *perfect* dislocation (b)- the phason singularities (there are many attached to each $\mathbf{b}_{||}$-dislocation), that we call *matching faults*, are *dipoles of dislocations* whose Burgers vectors are of a special type; they do break not only a particular symmetry of translation but also the *class of local isomorphism* (in the jargon of QCs) of the QC. In fact, such dipoles, if they open up into loops, bound *stacking faults* – thus a phason singularity is an *imperfect* dislocation. A *mismatch* is nothing else than an elementary matching fault.

It is suggested that it is the simultaneous presence of perfect dislocations and of phason singularities, and their interplay, that are at the origin of the peculiar characters of the plastic deformation of quasicrystals, namely the brittle-ductile transition followed by a stage of work softening; in particular the brittle-ductile transition could be related to a cooperative transition of the Kosterlitz-Thouless type which affects the dipoles and turn them into (imperfect) dislocation loops.

1-INTRODUCTION

The investigations of the plastic deformation properties of quasicrystals have been marked in the last decade by a number of experimental and theoretical advances, but there are still a number of open questions.

A most intriguing one relates to the nature and role of phasons and phason defects, and to their interplay with phonon defects. This question has been attacked by various methods (simulations [1], topological classification of defects [2], phason variables measurements in function of the deformation [3], etc...). As it is well known, one observes in QCs the simultaneous presence of two types of strain, phonon (elastic) strains, as in usual crystals, and phason strains, that are specific of quasicrystals. As a consequence, one expects specific plastic deformation properties in QCs. From that point of view, it is difficult to say that the results do not come up with expectations. For example, most QCs show a very remarkable brittle-ductile transition (BDT) at a temperature T@0.7

TBDT, followed above TBDT by a surprising softening behavior, reminiscent of the softening observed in metglasses [4]. These properties have been dealt with by a number of authors (for a review, see Urban *et al.*, [3]), but not in the context of the present work, which bears mostly on the relations between dislocations and phason defects.

In this paper, the term of *dislocations* will be restricted to the singularities of the former type of strain, phonon strain; dislocations break (quasi)*translation symmetries*, as in usual crystals. *Matching faults* (as we shall venture to call the phason defects alluded to above) are the singularities of the latter type of strain, phason strain; we shall argue that they break, in a sense that will be defined, the *class of local isomorphism* (LI). This property is deeply related to the fact that matching faults can also be considered as (imperfect) dislocation loops or dipoles. We finally briefly discuss some features of the plastic behavior of quasicrystals.

Quasicrystallography theory can be presented in several ways: multigrid methods, projections from or intersections of higher space hyperlattices, etc.... In the latter mentioned type of presentation, one starts from a d-dimensional hyperlattice in an euclidean space E_d (*e.g.*, icosahedral case, d = 6; pentagonal – Penrose – case, d = 5; octagonal case, d = 4; in all three cases the hyperlattice is cubic; this is not the only possibility). The physical space $P_{||}$ of the quasicrystal is a $d_{||}$−plane in E_d, oriented along a direction that is irrational with respect to the hyperlattice. This latter condition means that $P_{\|}$ contains at most one node of the hypercubic lattice. The flat space E_d in which the hyperlattice is embedded is the Cartesian product $E_d = P_{||}$ Ä $P_{\wedge}$, where $P_{\wedge}$ is a flat space *perpendicular* to $P_{||}$; $d_{||} = d_{\wedge} = d/2$ in the icosahedral and octagonal cases. The atomic positions in the quasicrystal are defined as the *intersections* of $P_{||}$ with sets of congruent $d_{\wedge}$-dimensional *atomic surfaces* (AS) that are attached periodically to the hypercells (each set, which is globally invariant by the elements of the icosahedral, pentagonal or octagonal group, corresponding to a fixed Wyckoff position of an atomic species). Any AS belongs to a local copy of $P_{\wedge}$. For more details, see *e. g.*, the articles collected by Steinhardt and Ostlund [5], and for applications to realistic cases, Katz and Gratias [6].

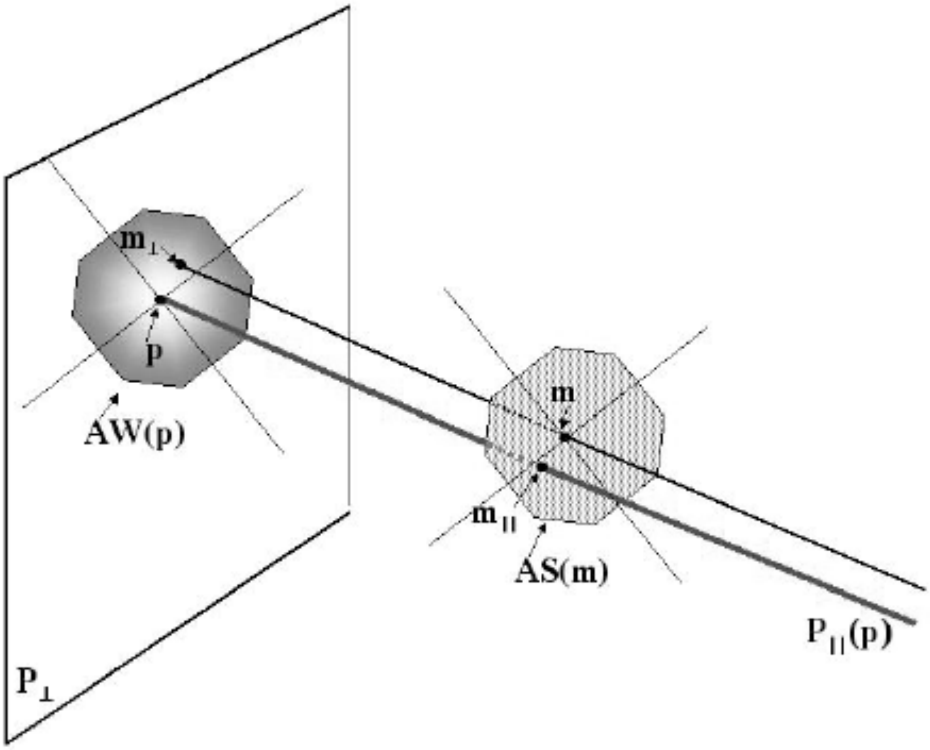


Fig. 1: Octagonal symmetry, d= 4. The 2-dimensional perpendicular plane $P_{\wedge}$ is fully represented (in perspective), whereas the 2-dimensional physical plane $P_{||}(p)$ which projects on $P_{\wedge}$ at a point p, is represented as a line which intersects the acceptance window AW(p) in its center. AW is the closure of the projections $m_{\wedge}$ of the hypercubic cells centers whose attached AS(m) intersect $P_{||}$. One of the AS(m)s is schematically represented. The projections $m_{\wedge}$ fill AW densely.

For the sake of clarity, we shall assume in the following that the hyperlattice is primitive (thus there is only one set of ASs), and each AS is taken equal to the projection of the hypercubic cell on $P_{\wedge}$ and is attached to each cell in such a way that the center of the cell m and the center of the atomic surface AS(m) coincide. Two ASs have no point in common; they can be brought into coincidence by a translation **b** of the hyperlattice. This simple model has been used by a number of authors; see e.g., [7] for octagonal ($d_{||} = 2$, $d_{\wedge} = 2$), Penrose ($d_{||} = 2$, $d_{\wedge} = 3$), and icosahedral ($d_{||} = 3$, $d_{\wedge} = 3$) QCs. Fig. 1 illustrates in a certain manner (see caption) the situation in the octagonal case.

The grid method will be succinctly presented below for the 2D Penrose tiling.

2-DISLOCATIONS AND MATCHING FAULTS: A REMINDER.

Dislocation hyperlines (hyperdislocations) in E_d are (d – 2)-dimensional manifolds [8], their Burgers vectors are lattice constants $\mathbf{b} = \mathbf{b}_{||} + \mathbf{b}_{\wedge}$. We restrict to hyperlines L that are the Cartesian products of $P_{\wedge}$ by their intersection $L_{||}$ with $P_{||}$, namely:

$L = L_{||}$ Ä $P_{\wedge}$; (1)

$L_{||}$ is the physical dislocation line. This decomposition has two advantages: (a)- if L could take any shape, the core would necessarily be anisotropic and extremely large compared to atomic dimensions [9], see Fig. 2; (b)- the shape of the dislocation line does not change under the effect of a uniform phason displacement [10].

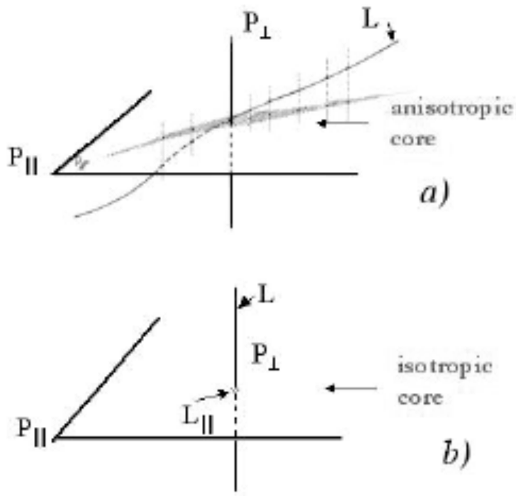


Fig. 2 Schematic representation of a dislocation in a quasicrystal. Illustration for $d_{\wedge} = 1$, $d_{||} = 2$; (point dislocation). (a)- The hyperline perpendicular to $P_{||}$, i.e., along a copy of $P_{\wedge}$, has a isotropic core; $L = L_{||}$ Ä $P_{\wedge}$; (b)- The core of a dislocation is necessarily anisotropic or extremely large compared to atomic dimensions, if L takes any shape.

Hyperdislocations are topological defects classified by the classes of loops of the order parameter space of the hypercubic crystal, specifically the first homotopy group $\text{p}_1(T_d) = Z^d$ of the d-dimensional torus T_d. The physical image in the QC of an hyperdislocation in E_d consists not only of the hyperdislocation intersection with $P_{||}$, *i.e.,* a physical dislocation, but also of a cloud of singularities of the phason variables, namely the matching faults alluded to above.

Observe that a measurement of the phonon strain field $\text{Ñ}_{||}\mathbf{u}_{||}$ made along a Burgers circuit surrounding $L_{||}$ in $P_{||}$ cannot yield anything else than $\mathbf{b}_{||}$ (= $\text{ò}d\mathbf{u}_{||}$), because $\mathbf{b}_{\wedge}$ does not belong to the physical space $P_{||}$. Hence $L_{||}$ is, in the usual sense, a true dislocation line with Burgers vector $\mathbf{b}_{||}$. The perpendicular component $\mathbf{b}_{\wedge}$ shows itself in $P_{\wedge}$ through a displacement field $\mathbf{u}_{\wedge}$, which affects the position of a certain number of atomic surfaces with respect to $P_{||}$, resulting in localized shifts of some atoms in $P_{||}$. The picture of the physical effect of $\mathbf{b}_{\wedge}$ which emerges from the above is somewhat complex, and this paper is to make it more accessible, hopefully. For this purpose, we do not use the continuous picture of the phason strain $\text{Ñ}_{||}\mathbf{u}_{\wedge}$, but its discrete version, which is in terms of *tilings*.

In the 2D Penrose tiling (PT), an atomic, localized, phason strain is represented by the *local shift* (or *flip*) of a node of the tiling, to the effect that two opposite edges of a large rhombus match wrongly with their neighbors (local matching rules are broken along *two mismatches*), see fig. 3.

We emphasize that it is necessary, when speaking of phasons, to clearly distinguish between an *atomic flip* and a *mismatch*: two mismatches belonging to the same rhombus can move *independently* along a *worm* and get apart [11]. *A mismatch is by itself a topological defect*, because it cannot disappear on the spot. On the other hand, a localized shift, being the sum of two mismatches of opposite signs, can disappear on the spot; *a local shift is not a topological defect*, but a (discrete) element of the phason strain. A mismatch is a singularity of the *phason strain* field in the same sense that a dislocation is a singularity of the *phonon strain* field.

These mismatches (not the phason strains) are precisely the most simple defects representing the physical content of $\mathbf{b}_\wedge$ [9]. They are elementary matching faults. But they also have an existence independent of the presence of a dislocation and can be considered as topological defects *per se*. Similarly, a dislocation of Burgers vector $\mathbf{b}_{||}$ can exist without being escorted by companion matching faults [12][1] . It is possible to attach a *topological invariant* to each mismatch, in the same way that it is possible to assign an (invariant) Burgers vector $\mathbf{b}_{||}$ to a dislocation. This has been shown [13] for mismatches in a PT belonging to the $g = 0$ LI class. We come back later to the notion of LI class, which is crucial for a full understanding of matching faults.

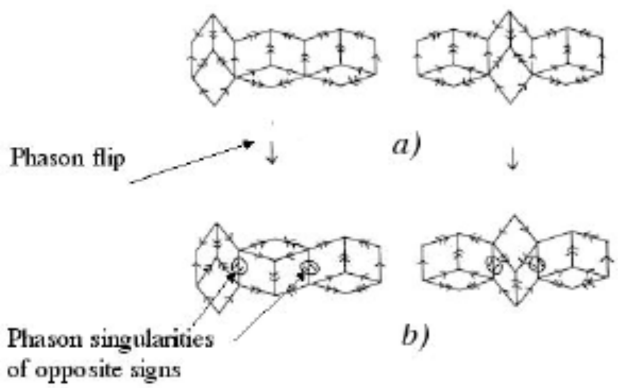


Fig. 3 Flip and mismatches of opposite signs in a PT. The two mismatches can diffuse apart by a process of consecutive local shifts. (a)- Perfect tiling along a row of 'hexagons'; (b)- Flip of a node in the central hexagon and appearance of two mismatches.

A more general approach to the topological theory of defects in QCs has been proposed [2]. We briefly mention it on account of a question of terminology. In the course of the development of the topological theory, the $d_\wedge$-dimensional projection $T_{d\wedge}$ of the d-dimensional torus T_d onto $P_\wedge$ does appear. T_d is the order parameter space (degeneracy space) of the d-dimensional crystal, and $T_{d\wedge}$ is the order parameter space of the quasicrystal. In analogy with the way T_d is related to the group of *translations* in the d-dimensional flat lattice (which is tiled by congruent T_ds), $T_{d\wedge}$ is related to the (non-commutative) group of *transvections* [14] in a $d_\wedge$-dimensional curved lattice (which is tiled by congruent $T_{d\wedge}$s). Hence the name of *disvections,* in analogy with *dislocations*. The group of translations classifies the **b**-hyperdislocations; the group of transvections classifies the $\mathbf{b}_{||}$-dislocations and the $\mathbf{b}_\wedge$-phason defects, all together. Because dislocations and phason singularities can be independent defects, we propose to restrict the use of the term of ‘matching fault’ to the latter defects (i.e. to the whole set of defects attached to the $\mathbf{b}_\wedge$ vector), the term of ‘dislocation’ (Burgers vector $\mathbf{b}_{||}$) keeping its usual meaning. ‘Disvection’, which gathers both types of defects, is the catchword for the *image* in the physical space $P_{||}$ of the hyperdislocation L of Burgers vector $\mathbf{b}$ in E_d.

3-MATCHING FAULTS IN A PENROSE TILING

We discuss now a certain number of physical and structural properties which show, on one hand, how matching faults can be described as *dislocations dipoles*, on the other hand, how they relate to the concept of *class of local isomorphism*. This section is devoted to 2D Penrose tilings, for which the above characters of matching faults can be easily exhibited. The (more difficult) extension to other cases is discussed in sections 4 and 5.

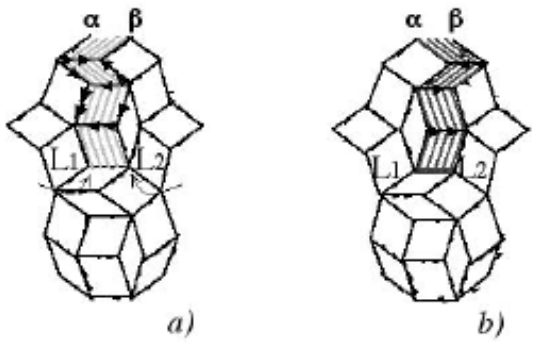


Fig. 4: PT: an elementary phason singularity as a *dislocation dipole*; $d_{||} = 2$, $d_\wedge = 3$. (a)-Cut surface along the polygonal line L_1a, removal of the line-patterned matter, glueing along L_1a - L_2b; these operations result in a dislocation +**b** in L_1 and a stacking fault along L_1a; (b) Cut surface along the line L_2b, addition of the line-patterned matter, glueing; these operations result in the disappearance of the L_1a and L_2b stacking faults (which are of opposite signs) and in a dislocation -**b** in L_2.

1- <u>*mismatches, dislocation dipoles*</u>

Mismatches are elementary matching faults: along edges in 2D QCs, along faces in 3D QCs. They can be considered as *imperfect dislocation dipoles*. This is illustrated Fig. 4 for a 2D PT belonging to the (usual) $g = 0$ LI class. The mismatch sits along L_1L_2 , and is the result of the mutual annihilation of two disvections at a lattice distance. The total Burgers vector of each (point) disvection forming the dipole is $\mathbf{b} = \mathbf{b}_{||} + \mathbf{b}_\wedge = \pm[1,0,0,0,0]$. But $\pm[1,0,0,0,0]$ is not a topologically stable Burgers vector of the PT [15]. In effect, the local configurations along the cut surface of any of these point disvections, L_1a say, are forbidden in the $g = 0$ LI class, and this situation cannot be healed by simple flips of the phason type, as we shall comment in more detail in the next subsection. We therefore refer to the cut surface ot the *imperfect* disvection as a *stacking fault*. On the other hand a topologically stable *perfect* disvection (*e.g.*, $\mathbf{b} = [1,-1,0,0,0]$) breaks the quasicrystalline translational symmetries, but does not break the LI class.

2– <u>classes of isomorphism</u>.

By definition, a *class of local isomorphism* contains a set of tilings that share the same set of finite subsets. The notion of LI class has been much studied in the first decade following the discovery of QCs [16, 17], but has since lost somewhat of its aura, probably because it is now believed that actual QCs of the same dimensionality and same symmetry all belong to the same class of isomorphism. The discussion which follows of the LI class of a PT is made in the frame of the grid dual method (GDM) developed by De Bruijn [18] and generalized in [19, 20].

(a)-*The grid dual method*. In the De Bruijn grid method, each mesh of the 2-grid is characterized by 5 integers k_i, each k_i increasing by one unit $k_i \rightarrow k_i + 1$ in the positive direction of the unit vector n_i perpendicular to the i-set of parallel lines forming the mesh, each time a line of the set is crossed. The n_is point along the edges of a regular pentagon. The PT is the dual of the grid, with nodes which can be written in complex coordinates $Z = \Sigma_i (k_i - \gamma_i) \xi^i$ for each mesh, where $\xi = \exp[2i\pi/5]$. The γ_is are arbitrary real numbers which define the origin of the grid.

The mesh is also the intersection of a 5D hypercubic lattice in E_5 with an irrational plane $P_{||}$. The equations of this plane are

$$\Sigma_i (x_i - \gamma_i) = 0 \qquad\qquad \Sigma_i (x_i - \gamma_i) \xi^{2i} = 0. \qquad (2)$$

The last equation stands for two equations in the field of real numbers. The order parameter which defines the LI class is $\gamma = \Sigma_i \gamma_i$. Each node of the PT is also the projection of a lattice node belonging to an hypercube intersecting $P_{||}$.

The integer $K = \Sigma_i k_i$ takes only a finite number of values, 4 values in a *true* PT, where $\gamma = 0$ (mod. 1), namely γ, $\gamma + 1$, $\gamma + 2$, $\gamma + 3$; K takes one value more in a *generalized* PT (γ noninteger), namely $\mathrm{Int}^+(\gamma)$, $\mathrm{Int}^+(\gamma + 1)$, $\mathrm{Int}^+(\gamma + 2)$, $\mathrm{Int}^+(\gamma + 3)$, $\mathrm{Int}^+(\gamma + 4)$, where $\mathrm{Int}^+(\gamma)$ is the smallest integer which is larger than γ.

(b)-*perfect and imperfect disvections* [15] Let us consider an disvection of Burgers vector $\mathbf{b} = \{n_i\}$, and introduce the scalar product $\mathbf{b}\cdot(1,1,1,1,1) = \Sigma_i n_i$, which is the projection of $\mathbf{b}$ on the five-fold axis perpendicular to $P_{||}$. If $\mathbf{b}\cdot(1,1,1,1,1) = 0$, one can convince oneself that the total variation of K along a loop surrounding it vanishes. The introduction of such a disvection does not modify the number of values taken by K. On the other hand, a disvection of the type $\mathbf{b}.(1,1,1,1,1) = \pm 1$ changes $K \rightarrow K \pm 1$ when traversing a closed loop; the number of values taken by K is now 5. We interpret this modification as follows. As a complete loop surrounding an disvection of Burgers vector $\mathbf{b}$ is traversed, γ_i changes to $\gamma_i + n_i$. The LI class is modified accordingly, $\gamma \rightarrow \gamma + \Sigma_i n_i$, where $\Sigma_i n_i$ is also $\mathbf{b}\cdot(1,1,1,1,1)$. Therefore the LI class takes all the intermediary values between γ and $\gamma + \Sigma_i n_i$ when the loop is traversed. There is no modification of the LI class if $\Sigma_i n_i = 0$, and the dislocation does not break the LI class. But it is broken if $\Sigma_i n_i \neq 0$.

The structural properties of the LI classes for $\gamma \neq 0$ have been studied by Pavlovitch *et al.* [21]. They show that a $\gamma \neq 0$ PT requires four types of tiles; the usual PT can be represented with only two types (two rhombi with a suitable arrowing of their edges), the density of supplementary tiles (the same rhombi, but differently arrowed) depending on the value of γ. A variable γ in a tiling can therefore be evidenced by the presence of a variable density of supplementary tiles whose arrowing fit with the arrowing of the original tiles, without the appearance of a discontinuity (a stacking fault) in the arrowing.

Coming back to the dipole of Fig. 4, observe that it is embedded in a g = 0 PT, but that the order parameter (the LI class) along the mismatch, which is what remains of the two stacking faults when they have merged, is different. The dipole is an imperfect disvection dipole. This is of little consequence as long as the distance between the two dislocation segments forming the dipole is comparable to the quasilattice parameter (*narrow* dipole). But if the dipole opens up into a dislocation loop, continuous variations of the g field between 0 and 1 have to show up along any Burgers circuit surrounding the dislocation. In the narrow dipole 'state' of the dislocation loop, those variations are amassed in the core of the mismatch; they form the mismatch itself.

To summarize, perfect translation defects in a PT, with å$_i b_i$ = 0, leave invariant the LI class g. In all other cases the notion of defect does subsist, but matching faults are no longer well defined. In fact, if no interest is taken in phason defects, the concept of LI class looses interest, and the Burgers vectors of *translation* defects can take values in the full range **b** = {n_i}, n_i Î Z, i =1,2,...,5. This is true in particular if phason flips , mismatches (and matching faults) have negligible energy; in that case the LI class is no longer a relevant observable.

4-MATCHING FAULTS AS DISLOCATION DIPOLES

The embedding of PTs in a d = 5 hyperspace is somewhat special, because it is possible to tune the LI classes by varying the projection of $P_{||}$ along the 5-fold axis (1,1,1,1,1). The grid method, as we have seen, gives a particularly transparent way of exhibiting the different LI classes. The icosahedral case (d = 6) and the octagonal case (d = 4) do not offer such a possibility: the LI class is unique, whatever the choice of the position of $P_{||}$. One can therefore wonder whether the same type of result holds, namely that mismatches, and more generally matching faults, are imperfect dislocation dipoles.

We show in this section that a phason singularity is an imperfect dislocation dipole in all QCs, not only PTs, irrespective of their symmetries and dimensionalities. The method in use, a detailed geometric study of the Volterra process (VP) for a disvection $\mathbf{b} = \mathbf{b}_\wedge + \mathbf{b}_{||}$, will let appear how $\mathbf{b}_\wedge$ matching faults are related to the perfect $\mathbf{b}_{||}$ dislocation.

1- *Cut surfaces in* E_d *and in* $P_{||}$

Let S be the cut surface in E_d of a hyperdislocation L, Burgers vector **b**. S intersects $P_{||}$ along $S_{||}$, which is the cut surface of $L_{||}$, in physical space. Generically, dim(S) = (d − 1), dim($S_{||}$) = ($d_{||}$ − 1). We know that the result of the VP in an usual crystal – which the hyperlattice is – does not depend on the choice of the cut surface. Then, instead of employing an arbitrary S in E_d, which would yield an arbitrary $S_{||}$, let us start from a $S_{||}$ chosen on purpose, and construct a S from such a $S_{||}$. It appears useful in a first step to start from a planar $L_{||}$ loop, whose plane contains the Burgers vector $\mathbf{b}_{||}$; $S_{||}$ is taken in the same plane. The advantage of this choice is that the VP does not require any addition or removal of matter in physical space, a process that would be difficult to analyze in a quasicrystal[2]. The same results obtain if $S_{||}$ is a cylindrical surface parallel to $\mathbf{b}_{||}$, and $L_{||}$ a closed line inscribed on the cylinder. Such restrictions can be removed later on, by reshaping the loop by glide and climb (and possibly diffusion for matching faults). The choice of $L_{||}$ and $S_{||}$ is also done in such a way that $S_{||}$ contains a high density of atomic sites $m_{||}$ of the QC. Let $S_{||}^{+}$ and $S_{||}^{-}$ be the lips of the cut surface. In the VP, we shall displace one lip, $S_{||}^{+}$, say, by a vector **b** relatively to the other, namely $S_{||}^{-}$, which stays fixed. We do not specify to which lip $S_{||}^{+}$ or $S_{||}^{-}$ the atomic sites $m_{||}$ do belong: rather, when the VP is turned on, we consider that each atom belonging to $S_{||}$ is split into two copies, one dragged by the movement of $S_{||}^{+}$, the other one staying in place in $S_{||}^{-}$. When the VP is completed, certain atoms on $S_{||}^{+}$ coincide with atoms on $S_{||}^{-}$; those atoms are then identified. This is precisely what one would do in a classic VP, for a perfect dislocation, in a classic crystal. But because we are dealing with a QC, other atoms do not hit an occupied site. This is where the phasons play a role, as we discuss in some detail.

It would be nice to have a S in E_d with properties akin to those of $S_{||}$, *i.e*. such that it contains the Burgers vector **b** and the hyperlattice centers from which the atomic sites in the QC are derived, as intersections $m_{||}$ of the *atomic surfaces* AS(m) attached to each hyperlattice center m: $m \rightarrow m_{||}$. To get this result, it is sufficient to take for S the Cartesian product of $S_{||}$ by $P_{\perp}$,

$$S = S_{||} \otimes P_{\perp}, \qquad (3)$$

in complete analogy with our choice for $L = L_{||} \otimes P_{\perp}$, Eq. 1.

We indicate some properties attached to our choice for S and $S_{||}$:

(i)- the copy of $P_{\perp}$ attached to $m_{||}$ belongs to S; it contains AS(m) and m. Hence AS(m) belongs to S.

(ii)- since $\mathbf{b}_{\perp}$ and $\mathbf{b}_{||}$ both belong to S, the full Burgers vector **b** belongs to S. The VP does not require removal or addition of matter in the high-dimensional space. Let us notice, in passing, that such a S is not generic. But again, the final result in the d-dimensional space does not depend on the choice of S.

(iii)- because any AS(m) in E_d belongs to a copy of $P_{\perp}$ (call it $P_{\perp}$(m)), it is either entirely in S or has no point in common with S. If a AS(m) has one point in common with S, it also has a point in common with $S_{||}$. Observe that AS(m) may belong to a $P_{\perp}$(m) which intersects $S_{||}$, but the intersection is not necessarily a point of AS(m).

(iv)- let $m_{||}$ be an atomic site on $S_{||}^{+}$; m belongs to S, according to (i)-. The displaced site m' = m + **b** is also in S, since **b** is in S. But AS(m'), which belongs to S, does not necessarily intersect $S_{||}$.

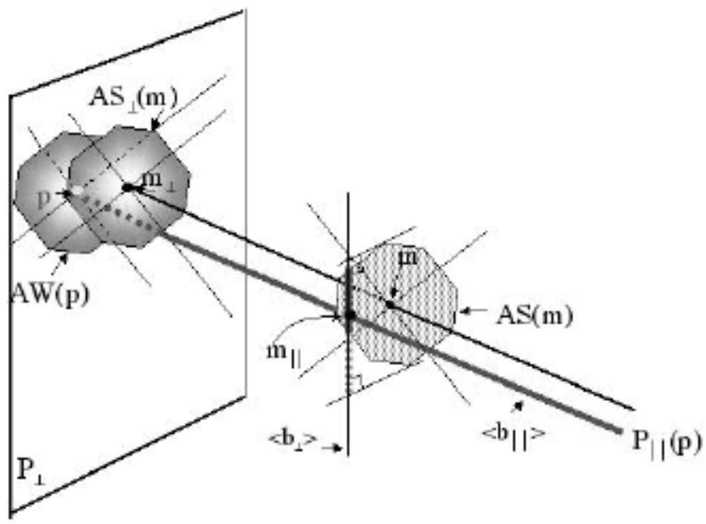


Fig. 5: Embedding of the plane $P^2(m_{||})$, defined by the directions<$\mathbf{b}_{||}$> and <$\mathbf{b}_\wedge$> in E_d and attached to $m_{||}$. Illustration for d = 4, octagonal symmetry; the 2-dimensional physical plane, which projects on $P_\wedge$ in one point, p, is represented as a line which is taken (in the drawing) along <$\mathbf{b}_{||}$>.

(v)- consider the set of parallel 2D planes which contain the two directions <$\mathbf{b}_\wedge$> and <$\mathbf{b}_{||}$>. The notation <**a**> designates the infinite line in the direction of **a**. We call $P^2(m_{||})$ the plane of this set attached to the atomic site $m_{||}$ in the physical space $P_{||}(p)$, <$\mathbf{b}_{||}(m_{||})$> the direction attached to $m_{||}$, see Fig. 5. If $m_{||}$ belongs to $S_{||}$, the vertical lines (along <$\mathbf{b}_\wedge$>) drawn from the intersection of <$\mathbf{b}_{||}(m_{||})$> with the dislocation line $L_{||}$ delimitate an infinite strip in $P^2(m_{||})$ which belongs to S.

Observe that in the $P^2(m_{||})$ plane, all the directions parallel to <$\mathbf{b}_{||}(m_{||})$> belong to a copy of $P_{||}$, all the directions parallel to <$\mathbf{b}_\wedge$> belong to a copy of $P_\wedge$. Because $P_{||}$ is perpendicular to $\mathbf{b}_\wedge$, the *intersection* of $P_{||}$ with P^2 is also the *projection* of $P_{||}$ on P^2, along <$\mathbf{b}_{||}$>. Similarly, the *intersection* of $P_\wedge$ with P^2 is also its *projection* on P^2, along <$\mathbf{b}_\wedge$>.

2-*The Volterra process; true and false sites*

We split the VP into two steps: (i) a displacement which, if first performed, brings any lattice site $m_{||}$ belonging to $S_{||}^+$ to $\mathsf{m}_{||} = m_{||} + \mathbf{b}_{||}$, and (ii) a displacement which brings $\mathsf{m}_{||}$ to $m_{||}' = \mathsf{m}_{||} + \mathbf{b}_\wedge$. We call these elementary VPs the $\mathbf{b}_{||}$-step and the $\mathbf{b}_\wedge$–step. The order in which they are performed is irrelevant. The site $m_{||}$ belongs to $P_{||}$; $m_{||}'$ belongs to another realization of the QC, $P_{||}'$. We discuss the geometrical features of the VP in the 2-plane P^2, see Fig. 6. Sites $m_{||}$ and $m_{||}'$ are *true* QC sites (for two different QC realizations), and are points belonging to two atomic surfaces AS(m) and AS(m'), such that m' = m + **b**. In E_d, the VP consists in a displacement m ® m', with a simultaneous transport of AS(m) to AS(m'). Now the question is whether $\mathsf{m}_{||}$ is true or false; (if a point in $P_{||}$ is not at an intersection with an atomic surface, we call it *false*).

If $m_{||}$ is *true*, its local environments carried by the two lips (above and below $S_{||}$) are in register along $S_{||}$, although the full local environment is not necessarily the same as for $m_{||}$. The VP so performed shows no difference with a usual VP for a perfect dislocation in a periodic crystal, but this resemblance is only local. We have achieved what can be called a *perfect* dislocation loop of Burgers vector $\mathbf{b}_{||}$; but the size of such a loop scales with the distance between neighboring atoms. If the same property could be repeated – but it cannot – for all the atoms on $S_{||}^{+}$, the local VPs on the cut surface would generate a set of contiguous perfect dislocation loops all of the same Burgers vector; this set, on the whole, would be equivalent to a dislocation along the loop $L_{||}$, of the same Burgers vector.

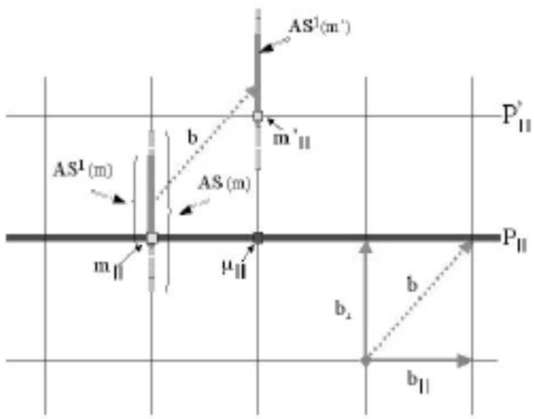


Fig. 6: Schematic representation of the VP displacement that affects a site $m_{||}$ in $S_{||}^{+}$. The sketch is made in the $P^2(m_{||})$ plane. Each AS(m), irrespective of the value of d, $d_{||}$, $d_{\wedge}$, intersects P^2 along a line segment $AS^1(m)$ whose direction is parallel to $<\mathbf{b}_{\wedge}>$. This intersection is not void if and only if $m_{\wedge}$ falls inside AW(p). The full atomic surface *projects* on P^2 along $<\mathbf{b}_{\wedge}>$. $AS^1(m)$ is represented as a full line and the projection of the rest of the AS as a line with a narrow horizontal pattern. See also Fig. 5. The atom formerly in site $m_{||}$ hits a site $m_{||} = m_{||} + \mathbf{b}_{||}$ which is empty (false site) in the present figure.

Fig. 6 illustrates the case when $m_{||}$ is *false*. This is the case alluded to above, where the VP does not work as in a usual crystal. The points of P^2 which are true sites for atoms in the different realizations of perfect QCs belong to the intersections of P^2 with all the atomic surfaces AS(m) attached to all the hyperlattice cell centers m. We call these intersections $AS^1(m)$; they consist in a segment of straight line.

Rule: $m_{||}$ (= m + $\mathbf{b}_{||}$) is *true* if and only if the vector $\mathbf{b}_{\wedge}$ whose head is taken in $m_{||}$ is entirely embedded in $AS^1(m)$, *i.e.*, in AS(m), as it is easy to see. This property is represented Fig. 7, for the octagonal case. The atomic surface of Fig. 7 is a generic AS which contains all the possible $m_{||}$ sites. It is divided into two domains, one relative to true sites (I), the other one to wrong sites (II).

3-<u>*The extension of the Volterra process for false sites*</u>

We show in this section how the Volterra process has to be modified when the site is false. The fundamental result is that one has to replace locally the perfect disvection **b** by an imperfect disvection $\mathbf{b}_{disv} = \mathbf{b}_{||}^{*} + \mathbf{b}_{||}$. The perpendicular component of $\mathbf{b}_{disv}$ vanishes, so that this disvection reduces to an imperfect dislocation (a matching fault); $\mathbf{b}_{||}$* is a Burgers vector (in the sense that it is still a projection of a hyperlattice vector **b***) which depends on $m_{||}$ but belongs to a restricted set of vectors, which we call *flipping vectors*, and which are the vectors which join the centers of two adjacent hypercells. These flipping vectors relate to the flips described since long in QCs. They also relate to the different types of stuctural modifications of the quasicrystalline arrangements in a matching fault. The reason of a special VP for false sites is of physical origin: the modified VP preserves the density of atoms. The detailed demonstration goes as follows.

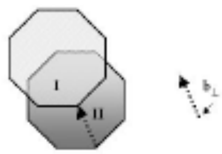


Fig. 7: For the $\mathbf{b}_\wedge$ vector indicated, the atomic surface for the $m_{½½}$ projections of m divides into two regions. Region I (which is the intersection of AW and the AW translated by $\mathbf{b}_\wedge$)): the $m_{½½}$ sites are true; Region II: the $m_{½½}$ sites are false.

If $m_{||}$ is *false*, one immediately notices that, by filling $m_{||}$ with an atom, as a result of VP, increases the local density, if another atom near-by is not removed. What happens in the course of the VP in this case can be understood as follows.

Consider, Fig. 8, two atomic surfaces AS(m) and AS(m*) which have a common $d_{||}$-dimensional tangent plane, parallel to $P_{||}$, denoted P(m,m*) (the so-called *silhouetting tangent plane* [7]). We claim that it is this geometry that is at the origin of the discontinuous *flips* in a quasicrystal: if AS(m) is displaced in such a way that it looses its intersection $m_{||}$ with $P_{||}$, another AS(m*) hits $P_{||}$ and enters it, at the moment $m_{||}$ leaves it (this is how the number of atoms is preserved). The phenomenon is illustrated in Fig. 8 for the octagonal case: the two hypercubes (not drawn), which project on the perpendicular space along $AS_\wedge$(m) and $AS_\wedge$(m*), have a common edge in E_d (not represented), from which can be drawn physical planes (copies of $P_{||}$) which do not penetrate the two hypercubes (since they fall on the common edge of $AS_\wedge$(m) and $AS_\wedge$(m*) in $P_\wedge$). The lifts AS(m) and AS(m*) — the atomic surfaces — of $AS_\wedge$(m) and $AS_\wedge$(m*) in E_d have no point in common.

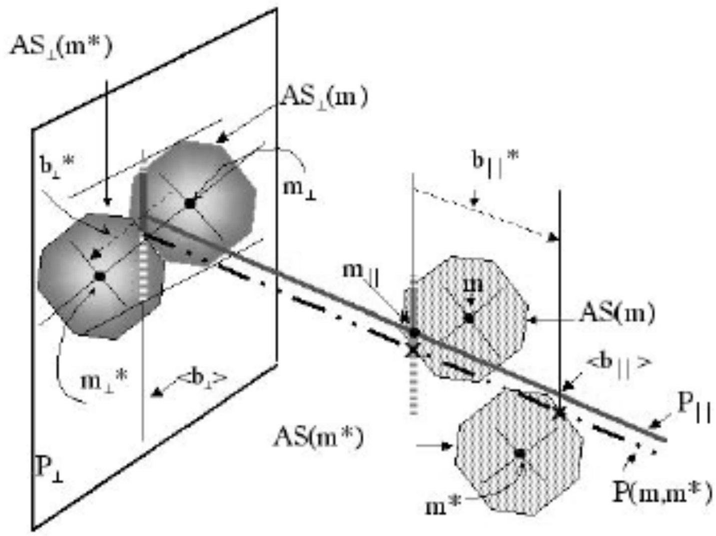


Fig. 8: AS(m) and AS(m*) are tangent along a 1-face (more generally, a ($d_\wedge$- 1) face), as well as their projections AS($m_\wedge$) and AS($m_\wedge$*) on $P_\wedge$. The ASs are centered in E_d on the centers m, m* of the hypercubes; m and m* project on $m_\wedge$ and $m_\wedge$* on the perpendicular plane. Let m* = m + **b***, with **b*** = $\mathbf{b}_\wedge$* + $\mathbf{b}_{||}$*. Notice that the representation of $\mathbf{b}_\wedge$* is easy, because $P_\wedge$ is represented with its full dimensionality (although in perspective); but $\mathbf{b}_{||}$*, which belongs to a $P^2(m_{||}*)$ plane different from $P^2(m_{||})$, generically, is not represented. P(m,m*) is called a *silhouetting tangent plane*.

Now, when AS(m) moves along <$\mathbf{b}_\wedge$>, and if one assumes that AS(m*) experiences the same motion, then AS(m*) enters $P_{||}(p)$, at the very moment when AS(m) leaves it: a flip happens, $m_{||}$ ® $m_{||}$*, where $m_{||}$* is the projection of AS(m*) onto $P_{||}$. This geometry is most easily represented in the $P^2(m_{||})$ plane, Fig. 9. Note that $m_{||}$* does not depend on the magnitude of the displacement along <$\mathbf{b}_\wedge$>, but $m_{||}$* = $m_{||}$ + $\mathbf{b}_{||}$* is defined unambiguously.

In the above analysis of the flip, we have made the assumption that the atomic surfaces AS(m) and AS(m*) are both moving. Now we prove that this is indeed the case in the VP. We select the tangent plane at the extremity of AS^1(m) which is opposite to the facet crossed by $m_{||}$ during the $\mathbf{b}_\wedge$-step (we perform the $\mathbf{b}_\wedge$-step before the $\mathbf{b}_{||}$-step). AS(m*) is then unambiguously determined. We employ the specific features that we have chosen for the cut surfaces S and $S_{||}$. An essential property of AS(m*) is that it *does* belong to S. In effect, even if $m_{||}$* = $m_{||}$ + $\mathbf{b}_{||}$* is not in $S_{||}$, generically, because $\mathbf{b}_{||}$*

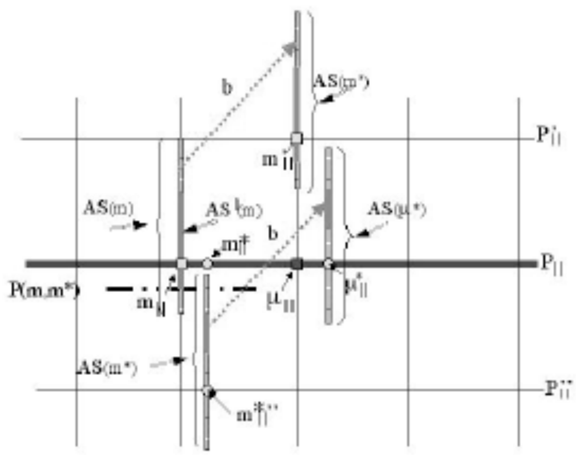


Fig. 9: The Volterra process completed for a site $m_{||}$ which hits a false site $m_{||}$ in the translation $m_{||} = m_{||} + \mathbf{b}_{||}$. Because of the 'shift' which occurs during VP between AS(m) and AS(m*), the final transform of $m_{||}$ in the process is $m_{||}$*. See text.

is not generically in $S_{||}$, m* belongs to S, because it is at a small, atomic, distance from m, and its projection on $P^2(m_{||})$ is therefore inside the strip, defined above section 4.1, bound by the intersection of the dislocation L with $P^2(m_{||})$. Therefore AS(m*) is indeed dragged along with AS(m) when the VP is progressing, even if the flip $m_{||}$ ® $m_{||}$* does not belong to VP, *stricto sensu*. The effect of the $\mathbf{b}_\wedge$-step is to replace $m_{||}$ by $m_{||}$* , the effect of the $\mathbf{b}_{||}$-step is to bring $m_{||}$* in the final position $m_{||}^* = m_{||} + \mathbf{b}_{||}^* + \mathbf{b}_{||}$. The total Burgers vector is

$$\mathbf{b}_{disv} = \mathbf{b}_{||}^* + \mathbf{b}_{||}. \qquad (4)$$

Another way to find this result is to notice that the displacement of AS(m) can be split into two parts, one which brings it to the former position of AS(m*), by a translation $\mathbf{b}_1 = \mathbf{b}_{||}^* - \mathbf{b}_\wedge$, then a second one from this position to AS(m*), by a translation $\mathbf{b}_2 = \mathbf{b} = \mathbf{b}_{||} + \mathbf{b}_\wedge$, One gets $\mathbf{b}_1 + \mathbf{b}_2 = \mathbf{b}_{disv}$. The $\mathbf{b}_1$-step can be considered as a relaxation process that insures that the atomic density is constant. We have created locally, through a very unusual VP, whose physical Burgers vector is $\mathbf{b}_{||}^* + \mathbf{b}_{||}$, whose perpendicular vector vanishes. Clearly, the total Burgers vector $\mathbf{b}_{disv}$ is not a valid Burgers vector of the QC. The dislocation of Burgers vector $\mathbf{b}_{disv}$ is imperfect and carries a stacking fault. We characterize it more fully in the next section.

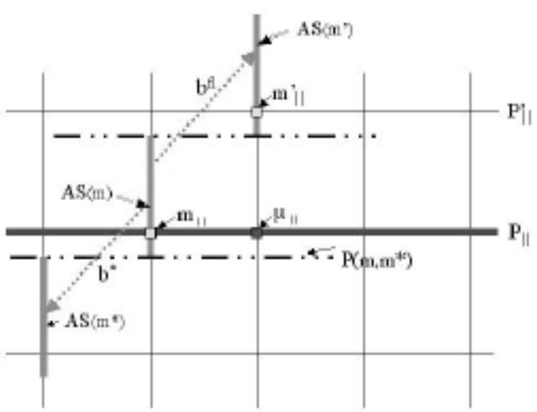
5-IMPERFECT DISLOCATIONS IN QCS

1- <u>*Flipping Burgers vectors and pure matching faults*</u>

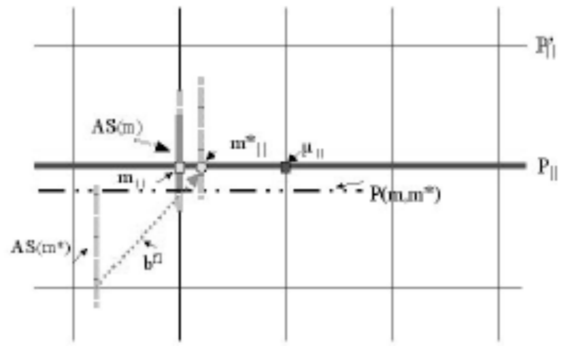
The subset of all Burgers vectors $\mathbf{b}^{fl} = \mathbf{b}_{||}^{fl} + \mathbf{b}_\wedge^{fl}$ which join the centers of two hypercubes in contact along a silhouetting face – we call them *flipping* Burgers vectors – yields in physical space disvections of a particular nature (the **b*** vector in the latter section was a flipping vector). Before developing this point, we first emphasize the special characters of these Burgers vectors.

Flipping Burgers vectors are related to the *silhouetting* $d_{||}$-dimensional directions introduced in [7]. The term *silhouetting* [7] is self-explanatory; it refers to all the physical planes $P_{||}$ which are tangent to two hypercubic cells which have a ($d_\wedge$ − 1)-dimensional face in common, *i.e.*, a 2-face for the icosahedral QC ($d = 6$, $d_\wedge = 3$) and the Penrose tiling ($d = 5$, $d_\wedge = 3$), a 1-face (an edge) for the octagonal QC. In the simplified model of the QC that we are investigating, if one chooses for all the congruent ASs the projection of an hypercube onto $P_\wedge$, the silhouetting directions of neighboring hypercubes having a ($d_\wedge$ − 1)-face in common shape a right cylinder around each AS, each generatrix of this cylinder being a $P_{||}$. The vector $\mathbf{b}^{fl}$ is precisely the vector which joins the centers of two hypercubes which have a face in common. A complete table of the $\mathbf{b}^{fl}$s for icosahedral and Penrose QCs can be found in [7].

Consider now a disvection of Burgers vector $\mathbf{b}^{fl} = \mathbf{b}_{||}{}^{fl} + \mathbf{b}_\wedge{}^{fl}$. In the corresponding 2-plane P^2 at $m_{||}$, Fig. 10a), b), the projection AS^p of any AS has a length exactly equal to $b_\wedge{}^{fl}$, but the length of the intersection AS^1 depends on the position of p inside $AS_\wedge(m)$. This is illustrated Fig. 11 and discussed later on. But first a remark: it is easy to convince oneself that, whatever the position of $AS^p(m)$ and the length of $AS^1(m)$ may be along $<\mathbf{b}_\wedge{}^f>$, $m_{||}{}^{fl}$ is false, except in the limit case when m meets two conditions, (i)- $AS^1(m) = AS^p(m)$, (ii)- AS(m) is tangent from below to the physical plane. But such ms are exceptional. Consider then the generic case, and call $\mathbf{b}^*$ (as in the latter section) the flipping vector: the construction discussed in the former section consists in finding an AS(m*) that is tangent to P(m,m*), at a vector distance $\mathbf{b}^*$. We have two cases.



***a*)**



b)

Fig. 10. The Volterra process for a flipping Burgers vector; $\mathbf{b}^{fl}$, as seen in the plane $P^2(m_{½½})$. a)- $AS^p(m) = AS^1(m)$, the projection and the intersection of AS(m) with $P^2(m_{½½})$ are equal Þ $\mathbf{b}^* = -\mathbf{b}^{fl}$; $\mathbf{b}_{disv} = \mathbf{0}$; b)- AS(m*) = AS(m) + **b***, **b*** ¹ $\mathbf{b}^{fl}$.

In the case when $AS^p = AS^1$, Fig. 10a), it is easy to see that it must be $\mathbf{b}^* = -\mathbf{b}^{fl}$, because the AS(m)s which intersect in this manner $P^2(m_{||})$ repeat periodically along the direction <**b**>. One then find $\mathbf{b}_{disv} = \mathbf{0}$; the corresponding matching fault vanishes.

But, in the cut surface $S_{||}$ of the same disvection $\mathbf{b}^{fl}$, there are generically other $m_{||}$ atomic sites that require other flipping vectors **b*** ¹ – $\mathbf{b}^{fl}$, Fig. 10b). Again, these

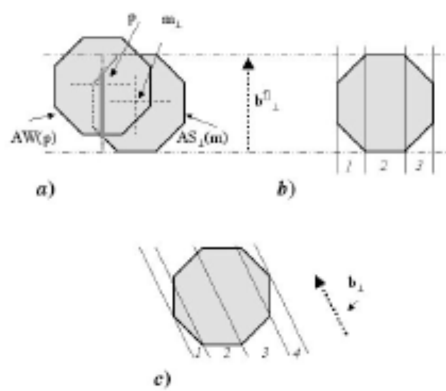


Fig. 11. Different types of flipping vectors in an octagonal quasicrystal. a) and b): The full disvection Burgers vector is itself a flipping vector: there are three possibilities, one of them (here type 2 in b)) yielding null matching faults; c) Generic case: there are four types of matching faults for the full dislocation $\mathbf{b} = \mathbf{b}_{½½} + \mathbf{b}_{\wedge}$.

occurrences are discussed in the next section. It is then Eq. 4 that must be used. In any case, a flipping disvection is entirely made of matching faults, if its cut surface $S_{||}$ is of the type defined above, namely parallel to $\mathbf{b}_{||}^{fl}$.

2-*The classification of matching faults*

Observe first that the direction <$\mathbf{b}_{\wedge}$> projected on $P_{\wedge}$ has a fixed point, the projection p of the physical plane on $P_{\wedge}$, Fig. 5 and 11; <$\mathbf{b}_{\wedge}$> is therefore a fixed direction in $P_{\wedge}$, for a given Burgers vector **b**. AS($m_\wedge$) moves in $P_\wedge$ in such a way that its center $m_\wedge$ remains inside AW(p); the lift of AS($m_\wedge$) in the corresponding hypercubic cell intersects the physical plane in $m_{||}$. We are interested in those $m_{||}$s that are on the cut surface $S_{||}$. The corresponding $m_\wedge$s form in $P_\wedge$ a discrete set that can be anywhere in AW(p), depending on the shape of the cut surface $S_{||}$. The location of $m_\wedge$ in AW(p) tells immediately (1)- whether the corresponding $m_{||}$ is true or false in the VP, (2) if $m_{||}$ is false, which face of AS($m_{||}$) is met by <$\mathbf{b}_\wedge$(p)> when the VP is performed, i.e. which flipping vector is to be used. Fig. 11a) and b) illustrate the situation for a disvection whose Burgers vector is a flipping vector: there are 3 faces which can be met (i.e. 3 types of matching faults) in an octagonal QC. Fig. 11c) illustrates the generic case; there are now 4 types of matching faults.

6-PENROSE TILINGS REVISITED. A UNIFIED VIEWPOINT

It is of course possible to describe the quasicrystallography of a PT as an irrational embedding of a $d_{||}$ = 2 physical plane in a 4D crystal, i.e. with $d_{||} = d_\wedge = d/2$, in analogy with the icosahedral case and the octagonal case discussed above. But, also in analogy, there is only one LI class made visible. Notice however, as a special property of the PT case, that the hyperlattice is no longer cubic, but rhombohedral [22], which makes the geometrical representation a little bit more tricky; this is the reason why the d=5 embedding is preferred. As shown in [7], there are 10 flipping vectors in d = 5, but it is easy to see that they project in the d = 4 subspace $P_{||}$ Ä $P_\wedge$ along 5 flipping vectors which are precisely along the projections of the 5 directions of the type {1,0,0,0,0}. The discussion of the matching faults of the PT in the d = 4 embedding then goes like the discussion of the matching faults of the icosahedral (d = 6) and the octagonal (d = 4) QCs.

Reciprocally, one can embed the icosahedral and the octagonal QCs, and indeed any QC, in a crystal of arbitrary dimension. This process would possibly visualize a wide range of LI classes, and also multiply the number of possible flipping vectors, *i.e.* the number of possible structures of mismatches (and of their corresponding matching faults). Now all such structures do not have the same free energy. This situation is reminiscent of what can be said of stacking faults in close-packed crystals. Consider, *e.g.*, a fcc stacking ...CABCABCABC.... A typical fault in the stacking, ... CABABCABC..., say, – resulting from a partial shift that we note $\mathbf{b}_{||}^{fl}$ – is such that the long distance interactions are modified with respect to the ground state, but preserves close-packing, so that the energy penalty is small. But a partial shift that does not preserve close-packing has a large energy, and is thus forbidden, or of a very small probability, at least. Similarly, one expects that the only mismatches which survive in a QC are those which do not deviate from a QC local symmetry. The standard embedding of a PT in a 5D crystal respects 5-fold symmetry; this is precisely why the number of flipping vectors effective for mismatches is 5, not 10. Any other embedding would yield high energy mismatches. Remarks of the same nature can be made for other QCs. The 12D embedding proposed in [19] preserves icosahedral symmetry and yields $\binom{d}{d_\perp - 1} = \binom{12}{8} = 15\times 33$ flipping vectors, but there are only 15 effective flipping vectors in 6D.

7-CONCLUSION. PLASTIC DEFORMATION PROPERTIES RELATED TO MATCHING FAULTS

The above discussion is essentially geometrical and structural. An important conclusion is that phason singularities in quasicrystals are of the same nature than stacking faults, and that these stacking faults are classified the same way the mismatches are, *i.e.*, by a special set of vectors, already considered in [7] as *silhouetting* vectors, but which also are *flipping* vectors, as we have shown. Because of these especial characters, we prefer to give to these stacking faults the name of *matching faults*. Matching faults are companion defects to dislocations, in a way that is not fully discussed in this article. The relation between dislocations and matching faults is an essential feature of QCs: it is a geometrical relation, symbolized by the unique Burgers vector **b** which links $\mathbf{b}_{||}$ and $\mathbf{b}_{\wedge}$ – in that sense the name of *disvection* finds a justification –; it is also a physical relation, because the companion matching faults of a dislocation are relaxation features of the stress field of the dislocation. This article is indeed restricted to the case where the cut surface of the $\mathbf{b}_{||}$-dislocation is a glide manifold, which implies very special dislocation loops; this suffices to study the general nature of the matching faults, but certainly not to understand the role of the interplay between dislocations of any shape and matching faults. Observe that the shape of the hyperdislocation in E_d is *a priori* enough to determine the phason singularities belonging to the related disvection, because, the hyperdislocation being a perfect dislocation, its deformation field does not depend on the precise cut surface attached to it (as long as one can affect a unique elasticity to the objects in E_d, from the knowledge of the elastic moduli in the physical space). Observe also that, because the energy of matching faults depend crucially on the nature of the faults, (classified by the flipping vectors), one should also expect that the shape of the dislocation in physical space depends self-consistently on the matching faults attached to it, so that dislocations of special types might be favored. These are problems for future investigations, which should then be devoted to the questions, among others, related to the deformation of a dislocation loop in physical space, namely the questions of glide, climb, and diffusion of matching faults.

We want now to end this article with a few simple, very speculative, remarks, related to the role of disvections in the plasticity of quasicrystals.

QCs under deformation show the following characters:

(a)- they all exhibit a remarkable brittle-ductile transition (BDT) at $T_{BDT} \approx 0.7T_m$, *i.e.*, dislocations are not mobile below T_{BDT}, at least under small stresses[3]. Quasicrystals are brittle at low temperature ($T < T_m$).

The brittle-ductile transition (BDT) is a phenomenon common to most materials. Various theories have been advanced, either relying on the existence of *thermally activated phenomena* (thermally activated generation of individual dislocations, or thermally activated mobility of interacting dislocations) or on the effect of *thermal fluctuations* acting cooperatively on dislocation dipoles, which suffer a growth and multiplication instability at some temperature depending on the elastic constants and the applied stress, after the manner of a Kosterlitz-Thouless (KT) transition [24].

The T_{BDT} in QCs does not depend significantly on the predeformation imposed to the specimen, according to E. Giacometti *et al*. [25]. This points toward the importance of matching faults as leading actors at the transition. They are frozen at low temperature. We speculate that they suddenly multiply, by some cooperative effect similar to that one advanced in [24] for dislocation dipoles in usual crystals. In that sense the dipolar character of matching faults has some importance. This is the first issue that seems worth considering in the light of the present theory.

(b)-The brittle domain: the dislocations do not move (this would be by glide, as one may expect at low temperature), because their motion has to oppose a considerable Peierls stress, which comprehends the lattice friction and the nucleation of phason defects, cf. a 1D calculation of the Peierls stress in [26]. Observe that there is no *geometrical* reason why phason defects should move if the *elastic* coupling between the phonon and phason terms vanish in the elastic free energy density. This is an assumption which has often been made, but which is probably too simplistic.

(c)- Stage of work hardening: The nucleation of matching faults in the wake of moving dislocations is probably difficult. It is interesting to notice that there is a stage of work hardening at the beginning of the stress-strain curve, in the ductile domain; which can be interpreted as a multiplication of dislocations *above* the BDT, a multiplication which is made easier by the presence of a number of phason defects which have nucleated cooperatively and haven't then created a large phason strain.

(d)- Above this work hardening stage, we speculate that the phason strain increases when the dislocations nucleate under deformation, in what we believe is a second step after the KT nucleation of phason defects. Guyot *et al*. [27] claim that it explains the considerable work softening, attended by a strong increase of the dislocation density with temperature and with applied (phonon) strain. This increase of the dislocation density has been analyzed by the Jülich group [3] as relating to a considerable increase of the density of dislocations with tiny physical Burgers vectors $\mathbf{b}_{||}$. Correlatively, the phasonic part of the Burgers vectors $\mathbf{b}_{\wedge}$ increases, *i.e*, the density of phason defects increases (the authors measure the phason strain). The multiplication of phason loops might be at the origin of the multiplication of imperfect dislocations that originate in the opening up of the matching faults.

Other questions have been considered, in various works, which should be revisited in the light of the exact nature of the matching faults attending a given dislocation. Among them is the question of the *splitting* of the core, which is favoured as soon as the nucleation of matching faults is easy, because the phason content (proportional to $\mathbf{b}_{\wedge}$) increases when $\mathbf{b}_{||}$ decreases. Reciprocally, if there are already many matching faults, not attached to specific dislocations, this may provoke dislocation splitting.

The usual model to explain work softening is that the dislocations move (by glide, by climb?) in the wake of each other. This motion requires the nucleation/absorption of fresh phason defects. It is not the fact that they are in the same wake that is relevant, it is the fact that in the wake, there are such phason defects. Wherever such phason defects exist, the same effect of easy motion should prevail.

ACKNOWLEDGMENTS I wish to thank the 'Max-Planck-Institut für Physik Komplexer Systeme', Dresden, Germany, where most of this work was done during the workshop on Topology in Condensed Matter Physics. I am also grateful to Dr V. Dmitrienko, Prof. J. Friedel, and Dr. D. Gratias, for fruitful comments and discussions.

REFERENCES

1. Dilger, C., Mikullah, R., Roth, J., and Trebin, H.-R., , *Phil. Mag*. **A75**, 425 (1997).
2. Kleman, M., *J. de Phys*. **51**, 2431(1990); *J. Phys. I, France* **2**, 69 (1992).
3. Urban, K., Feuerbacher, M., Wollgarten, M., Bartsch, M., and Messerschmidt, U., in *Physical Properties of Quasicrystals*, Stadnik, Z. M. ed., Solid State Science 126, Springer, 361 (1999).
4. Friedel, J., in *Proceed. of the 5th Intern. Conf. on Quasicrystals*, Janot, Ch., and Mosseri, R., eds., World Scientific, 5 (1995).
5. Steinhardt, P.J., and Ostlund, S., eds, *The Physics of Quasicrystals*, , World Scientific, Singapore(1987).
6. Katz, A., and Gratias, D., in *Lectures on Quasicrystals,* Hippert, D., and Gratias, D., ed., Les Éditions de Physique, Les Ulis, 187. (1994).

7. Frenkel, D. M., Henley, C. L., and Siggia, E. D., *Phys. Rev.*, **B34**, 3649 (1986).
8. Kleman, M., in *Proceed. Of the I.L.L./Codest Workshop on Quasicrystalline Materials*, Janot, Ch., and Dubois, J.M., eds., World Scientific, 318 (1988).
9. Kleman, M., and Sommers, Ch., , *Acta Metall. Mater.*, **39**, 287 (1991).
10. Caillard, D., Vandershaeve, G., Bresson, L., and Gratias, D., , *Phil. Mag.*, **A 80**, 237 (2000).
11. Pavlovitch, A., Gefen, Y., and Kleman, M., , *J. of Phys.* **A22,** 4347 (1989)
12. Baluc, N., Yu, D.P., and Kleman, M., *, Phil. Mag. Lett.*, **72,** 1 (1995).
13. Timirpashaev, T. Sh., *J. de Phys. France*, **5**, 300 (1995).
14. Cartan, E., , *Leçons sur la géométrie des espaces de Riemann*, Gauthier-Villars, Paris (1963).
15. Kleman, M., Gefen, Y., and Pavlovitch, A., , *Europh. Lett.*, **1**, 61 (1986).
16. Socolar, J. E. S., and Steinhardt, P. J., , *Phys. Rev.*, **B34**, 617 (1986).
17. Katz, A., in *Aperiodicity and Order*, Jaric, M. V., ed., Academic Press, **2**, 147 (1989).
18. De Bruijn, N. G., *Ned. Akad. Weten. Proc. Ser.*, **A43**, 39, 53 (1981).
19. Kramer, P., and Neri, R., *Acta Crystall.*, **A40**, 580 (1984).
20. Socolar, J. E. S., Steinhardt, P. J., and Levine, D., *Phys. Rev.*, **B32**, 5547 (1985).
21. Pavlovitch, A., and Kleman, M., *J. of Phys.* **A20**, 687 (1987).
22. Janssen, T., 1986, *Acta Cryst.*, **A42**, 261.
23. Fikar, J., Bonneville, J., Rabier, J., Baluc, N., Proult, A., Cordier, P., and Stretton, I., *MRS Symposium Proceedings on Quasicrystals*, **643**, K7.4.1-K7.4.6 (2001).
24. Khanta, M., and Vitek, V., *Acta mater.,* **45**, 4675 (1997).
25. Giacometti, E., Baluc, N., and Bonneville, J., in *MRS Symposium Proceedings on Quasicrystals*, Dubois, J.M., Thiel, A. P., Tsai, and Urban, K., eds., **553**, 295 (1999).
26. Tamura, R., Takeuchi, S. and Edagawa, K., *Mater. Sci. Engng.,* **A309-310**, 552 (2001).
27. Guyot, P. and Canova, G., *Phil. Mag.* **A 79,** 2815 (1999).

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[1] In an electron microscope observation, the two Burgers components of the hyperdislocation cannot be separated, if they both exist; they yield indeed an electronic phase shift $\mathbf{G}\cdot\mathbf{b} = \mathbf{g}_{||}\cdot\mathbf{b}_{||} + \mathbf{g}_{\wedge}\cdot\mathbf{b}_{\wedge}$, where $\mathbf{g}_{||}$ and $\mathbf{g}_{\wedge}$ are the components of the diffraction vector $\mathbf{G} = \mathbf{g}_{||} + \mathbf{g}_{\wedge}$.

[2] However, let us observe that the analysis of the dipolar character of a mismatch, made in section 3-1, uses cut surfaces L_1a and L_2b which are perpendicular to the Burgers vector $\mathbf{b}_{||}$. The simplicity of the process results from the following: a)- one considers a dipole, not a unique dislocation, b)-the displacement $\mathbf{b}_{||}$ is equal to the edge of a tile, and propagates along a 'worm', c)- the cut surfaces follow the meandering of the worm. These characters are specific of a mismatch, not of a general matching fault.

[3] But note that experiments carried on AlCuFe have revealed that dislocations are mobile under a high hydrostatic pressure [23].