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Scripta Materialia 49 (2003) 11–17
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Dislocation climb in icosahedral quasicrystals

D. Caillard [a], F. Mompiou [a], L. Bresson [b], D. Gratias [b,*]

[a] *CEMES-CNRS, 29, rue Jeanne Marvig B.P. 4347, 31055 Toulouse Cedex 4, France*
[b] *LEM-CNRS/ONERA, B.P. 72, 92322 Châtillon Cedex, France*

Accepted 24 March 2003

Abstract

We discuss here some arguments in favor of climb being the dominant mode of dislocation motion responsible for the plastic deformation of icosahedral quasicrystals.
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Keywords: Quasicrystal; Dislocation; Climb; Glide

1. Introduction

Dislocations in quasicrystals were theoretically predicted [1,2] shortly after their discovery [3,4]. It took however several years before the first transmission electron microscopy (TEM) observations came out in real icosahedral [5–8] and decagonal [9,10] phases. A large effort has since then been devoted to understanding the geometrical properties of these defects (see for instance [11–13]) and reformulate the elastic theory in the quasicrystalline context [14–18]. On the experimental side, substantial progress was made in the interpretation of out-of-constrast conditions of dislocations [19,20] that lead to the determination of large number of various Burgers vectors for dislocations observed in different quasicrystalline materials [21–27]. The demonstration that dislocations are responsible for the plastic deformation in icosahedral phases has been done by *in situ* experiments [28] on i-AlPdMn. From this and further experiments (see, for instance [29–33]), the idea has rapidly emerged that dislocations in quasicrystals essentially move by glide, an hypothesis that was supported by sophisticated computer simulations using molecular dynamics [34–36] on simple 2D and 3D tiling models. General reviews of the research field of dislocations in quasicrystals can be found in [2,37,38].

The idea that climb could in fact be the predominant mode in the dislocation motion in quasicrystals came out more recently from the concomitant experimental determination [41–44] of both Burgers vectors and motion planes in as-cast single grains of i-AlPdMn. Although these works were essentially performed on genuine dislocations induced by the constraints generated during the elaboration and cooling of the samples, they indicated that climb should be a key mechanism to deal with in the modeling of dislocations motion in quasicrystals. It is our main goal to

* Corresponding author. Tel.: +33-146734445; fax: +33-146734155.
E-mail address: gratias@onera.fr (D. Gratias).

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doi:10.1016/S1359-6462(03)00165-9

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show here through several different examples why climb appears, to our opinion, as the predominant mechanism of dislocation dynamics in quasicrystals.

2. Quasicrystal dislocation basics

2.1. Geometry

We use the context of perfect quasicrystals in the sense of the cut and project method. Dislocations (see Fig. 1(a)) can be defined as Volterra singularities in the very same spirit as for usual crystals but transposed to the N-dim periodic object. The dislocation is said *perfect* if its N-dim Burgers vector is a vector of the N-dim hyperlattice Λ.

Because the 3-dim cut, say $\mathbf{E}_{\parallel}$, is irrationally oriented with respect to Λ, a perfect dislocation Burgers vector has necessarily a non-zero component in the complementary $(N-3)$-dim perpendicular space, say $\mathbf{E}_{\perp}$. Choosing uppercase letters for defining vectors of the N-dim space and lowercase letters for vectors lying in $\mathbf{E}_{\parallel}$ and $\mathbf{E}_{\perp}$, we have $\vec{B} = \vec{b}_{\parallel} + \vec{b}_{\perp}$ with $\oint_{\mathscr{C}} \mathrm{d}\vec{U}(\vec{R}) = \vec{B}$ for any closed loop $\mathscr{C}$ surrounding the dislocation hyperline of dimension $N-2$. This hyperline eventually

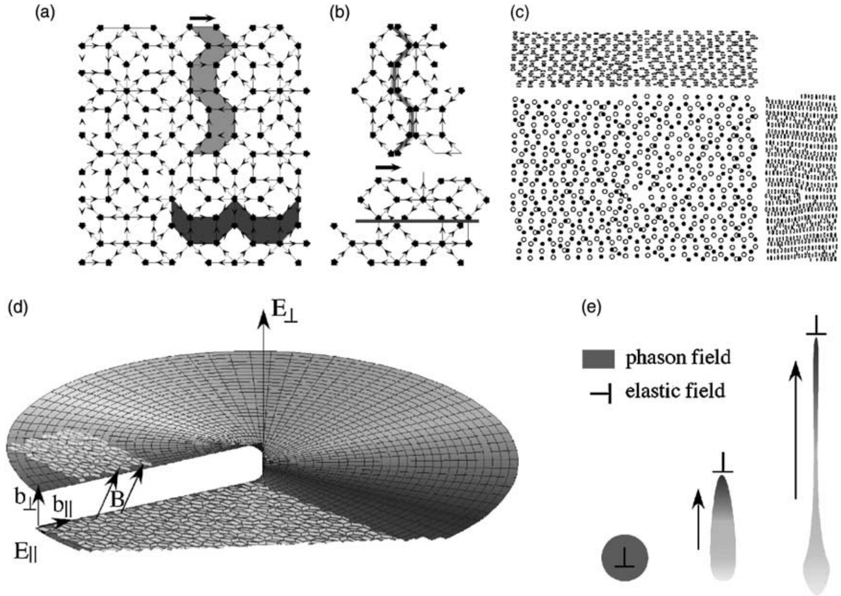

Fig. 1. (a) Example of how to generate a dislocation in an octagonal tiling: a cut along a worm (in gray) in the octagonal tiling generates a phason fault after translating along $\vec{b}_{\parallel} = (1,0,0,0)$. (b) There are two basic ways of displacing the tiling after the cut; on top the phason fault plane is chosen *perpendicular* to $\vec{b}_{\parallel}$, thus allowing a perfect match of the tiles *but inducing many matching rule violations*; in the bottom, the same displacement is performed but in a plane *parallel* to $\vec{b}_{\parallel}$. This does not allow for a geometric match of the initial tiles (irrespective of the matching rules). If we consider the worm as defining the motion plane of the dislocation, the former case corresponds to climb and the latter to glide. (c) A perfect dislocation in an icosahedral structure: thin slab of a F-type structure seen in 2-fold orientation built with two atomic surfaces (large triacontahedra) located at the even (○) and odd (●) vertices of a primitive 6D lattice. The Burgers vector is $B = (1,1,0,0,0,0)$. On the top and right sides, two views of this drawing at glancing angles show the dislocation core. (d) Metaphoric representation of a simple phason field $\vec{u}_{\perp}(\vec{r}_{\parallel})$ in the 2-dim octagonal tiling. Beside the standard deformation field (not shown), the dislocation creates a phason field that is equivalent to deforming correspondingly the physical space $\mathbf{E}_{\parallel}$ along $\mathbf{E}_{\perp}$. As for the elastic field, the phason field extends to infinity. (e) Schematic sketch of a dislocation moving by climb; the dislocation moves primarily under the action of $\vec{b}_{\parallel}$; a trailing phason fault is generated that progressively spreads out in the material by flip propagations depending on the speed of motion. In the case where the propagation speed is fast enough, an analysis of the leading dislocation line gives $\vec{b}_{\parallel}$ as Burgers vector with no component in $\mathbf{E}_{\perp}$. The N-dim nature of the Burgers vector of the dislocation is recovered by considering the complete object made of the dislocation line plus the phason fault.

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generates the dislocation line in $\mathbf{E}_{\parallel}$, the $(N-3)$ remaining dimensions are perpendicular to $\mathbf{E}_{\parallel}$, i.e. they are parallel to $\mathbf{E}_{\perp}$. Hence, for icosahedral quasicrystals, where $N=6$, dislocation hyperlines are 4-dim manifolds that decompose into one dimension in $\mathbf{E}_{\parallel}$—the actual dislocation line—plus three dimensions along $\mathbf{E}_{\perp}$. This geometrical construct is in agreement with the fact that the physical properties of the real dislocation should be independent of the choice of where the physical space $\mathbf{E}_{\parallel}$ hits [1] the perpendicular space $\mathbf{E}_{\perp}$. This, in turn, implies the displacement field $\vec{U}(\vec{R})$ to be independent of the perpendicular component of the running vector $\vec{R}$, i.e. $\vec{U}(\vec{R}) \equiv \vec{U}(\vec{r}_{\parallel})$. The perpendicular component $\vec{u}_{\perp}(\vec{r}_{\parallel})$ of $\vec{U}(\vec{r}_{\parallel})$ is a measure of the local shift of the physical space along $\mathbf{E}_{\perp}$, i.e. the phason field associated to the dislocation.

A convenient way for representing the dislocation phason field is given in Fig. 1(a) where a dislocation has been created in an octagonal tiling by removing a set of adjacent tiles along a vertical row (in grey)—called a worm in the tiling theory jargon—and translating the tiling along the horizontal common edge of the removed tiles (see Fig. 1(b), top). Although no new tile shapes have been created, the resulting object contains an extended defect called a phason fault in the sense that the matching rules (see Fig. 1(b), top) are violated all along the defect line (in gray in Fig. 1(b)), where new tile configurations have appeared that are not permitted in the perfect tiling. This extended defect can afterwards spread out more or less homogeneously in the tiling by successive flips of the hexagon configurations to partially recover correct local allowed configurations almost everywhere but in the neighborhood of the dislocation. This set of hexagon flips is equivalent to locally shifting the tiling along the perpendicular space (Fig. 1(c)), thus adding a perpendicular component $\vec{b}_{\perp}$ to the initial $\vec{b}_{\parallel}$ Burgers vector.

The way the phason field extends in the quasicrystal is determined by the displacement field $\vec{u}_{\perp}(\vec{r}_{\parallel})$ (see for instance Fig. 1(d)). For a closed circuit passing away from the dislocation core, the closure vector $\vec{b}_{\perp}$ in $\mathbf{E}_{\perp}$ is given by $\oint \mathrm{d}\vec{U}_{\perp}(\vec{r}_{\parallel}) = \vec{b}_{\perp}$. This shows that the linear phason density along a closed loop decreases as the inverse ratio of the distance from the dislocation core.

[1] Assuming that the hyperlattice Λ projects in an uniformly dense set of points in $\mathbf{E}_{\perp}$, as is the case in practice for icosahedral quasicrystals.

2.2. Dislocation motion

As previously said, dislocations are responsible for the plasticity of quasicrystals, because, as for ordinary crystals, they can move and interact with local and external stress fields mainly through their own elastic deformation field in $\mathbf{E}_{\parallel}$.

The question has raised to determine their motion modes according to the usual notions of glide and climb. A dislocation is said to glide if its Burgers vector in $\mathbf{E}_{\parallel}$ is in the plane of motion. This plane is the trace in $\mathbf{E}_{\parallel}$ of a $(N-1)$-dim hyperplane generated by the dislocation hyperline and the parallel component $\vec{b}_{\parallel}$ of the Burgers vector. On the contrary, a dislocation is said to climb if the parallel component $\vec{b}_{\parallel}$ of its Burger vector has a non-zero component outside the plane of motion. These two modes have clear physical meaning in crystals: glide corresponds to dislocation propagation with no long distance mass transport—taking advantage of the atomic periodicity in the crystallographic plane of motion—whereas climb is achieved by removing or adding matter in that plane, therefore requiring long distance atomic diffusion.

The situation is more tricky for quasicrystals. As the atomic structure of real quasicrystals can be reasonably well described as a decoration of template simple tilings (they are said to be in the same local derivability class), we observe that the simplest way to move a dislocation in such a tiling is to propagate a local collapse (or insert) of a worm of rhombi perpendicularly to the worm plane: this corresponds to the climb scheme in usual crystals. The process, examplified in Fig. 1(b) on the top, generates a phason wall in the motion plane but preserves the geometrical connections of the tiling. On the contrary, a shift parallel to the motion plane (corresponding to glide mode in crystals) destroys the local tiling by generating new tile shapes. In the N-dim picture, the first solution

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leads to a locally wavy but continuous $\mathbf{E}_{\parallel}$ manifold whereas the second solution generates a tear locally disrupting the $\mathbf{E}_{\parallel}$ manifold (see Fig. 1(b) bottom).

Hence, a major difference between climb and glide in quasicrystals is that, irrespective of the phason field redistribution that is common to both modes, climb motion can occur with no decohesion of the tiling whereas glide motion generates severe local damages in the tiling. This makes glide more suitable for the modeling of microcracks generation and propagation of microcracks rather than an easy dislocation motion as is usually the case in crystals. In both cases, phason reconstruction is equally required. But for climb, as in usual crystals, atomic diffusion to long distance is necessary to carry the excess (or loss) of matter during the move.

A rough scenario of the mechanisms of dislocation motion at high temperature could be the following. The dislocations move by climb under external stresses by reacting first to forces issued from the parallel component of the Burgers vector. This leaves a trailing phason fault bounded at its tail by a phason singularity $\vec{b}_{\perp}$. This extended fault can afterwards spread out around the dislocation core (see the sketch in Fig. 1(e)) once the dislocation has been immobilized.

3. Imaging dislocations using TEM contrast

The dislocation contrast observed by TEM are easily understood as for ordinary crystals within the column approximation. The clue point to notice here is that translating the cut space $\mathbf{E}_{\parallel}$ by $\vec{T} = \vec{t}_{\parallel} + \vec{t}_{\perp}$ of the N-dim space results in a phase shift of the Fourier coefficients $V_{\vec{T}}(\vec{G}) = V_0(\vec{G})\mathrm{e}^{2\mathrm{i}\pi\vec{G}\cdot\vec{T}} = V_0(\vec{G})\mathrm{e}^{2\mathrm{i}\pi(\vec{g}_{\parallel}\cdot\vec{t}_{\parallel}+\vec{g}_{\perp}\cdot\vec{t}_{\perp})}$, where $\vec{G} = \vec{g}_{\parallel} + \vec{g}_{\perp}$ are the wave vectors of the reciprocal N-dim lattice Λ^*.

Because of the above formula, all usual results obtained in crystals where the contrasts depend solely on phase changes in the Fourier terms of the potential (see for instance [39]) transpose exactly for quasicrystals as soon as the usual fault and diffraction vectors are replaced by their N-dim equivalents. In particular, contrast extinctions for a planar fault with fault vector $\vec{R}$ in N-dim are achieved once all active diffraction vectors $\vec{G}$ in N-dim are such that $\vec{G}\cdot\vec{R} = 0 \bmod 1$. For a dislocation of Burgers vector $\vec{B}$, this condition reduces to $\vec{G}\cdot\vec{B} = 0$ whatever the components of $\vec{B}$ in parallel and perpendicular spaces. These contrast rules have been established by Wollgarten et al. [40].

4. Experimental observations of dislocations in icosahedral quasicrystals

Dislocation contrasts and mode of motion have been studied by TEM in AlPdMn single grains. Results of *post mortem* observations, on as-grown samples (Section 4.1), on samples deformed at 300 °C under a high confining pressure (Section 4.2) and of in situ experiments (Section 4.3), reported in this section are extracted from Refs. [41–44] and from Mompiou et al. (to be published).

4.1. Perfect dislocations

Perfect dislocations have Burgers vectors that are translations of the 6-dim lattice. Strong extinctions for which $\vec{g}_{\parallel}\cdot\vec{b}_{\parallel} = \vec{g}_{\perp}\cdot\vec{b}_{\perp} = 0$ yield the Burgers vector directions in the physical and perpendicular spaces. Accordingly, the dislocations shown in Fig. 2 have Burgers vectors parallel to 2-fold directions out of the plane of motion—determined as the plane containing the (curved) line—in $\mathbf{E}_{\parallel}$, which shows that they have moved by climb. Weak extinctions are observed for $\vec{g}_{\parallel}\cdot\vec{b}_{\parallel} = -\vec{g}_{\perp}\cdot\vec{b}_{\perp}$. In those cases (see e.g. Fig. 2(c)), the phase shift of the strain field component compensates exactly that of the phason field. Fig. 2(d) shows that another diffraction vector parallel to the first one, but τ times longer in $\mathbf{E}_{\parallel}$, yields a normal contrast. In addition, strong residual contrasts are observed for large values of $\vec{g}\cdot(\vec{b}_{\parallel}\wedge\vec{u})$, where $\vec{u}$ is the unit vector parallel to the dislocation line. Single and double contrasts are also obtained for $\vec{G}\cdot\vec{B} = 1$ (Fig. 2(a)) and $\vec{G}\cdot\vec{B} = 2$ (Fig. 2(b)) respectively. These observations allow one to determine the Burgers vectors directions and lengths without ambiguity.

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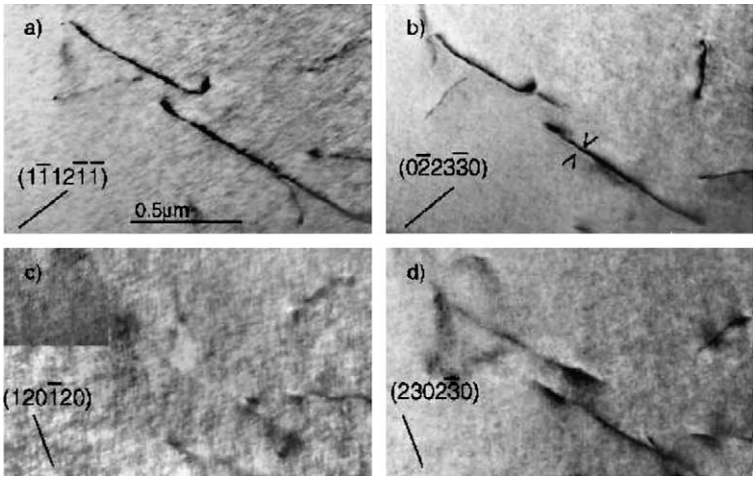

Fig. 2. Perfect dislocations in an as-grown AlPdMn single grain: (a) single contrast, (b) double contrast, ((c) and (d)) weak extinction and single contrast for two τ-related diffraction vectors.

4.2. Imperfect dislocations

Moving dislocations trail phason faults when the temperature is low enough to avoid fast phason dispersion. In their very definition, phason faults are characterised by a displacement vector $\vec{r}_\perp$ in $\mathbf{E}_\perp$. This vector can be equivalently written as $\vec{r}_\parallel = \vec{R} - \vec{r}_\perp$ in the physical space, where $\vec{R}$ is a vector of the hyperlattice, thus making them similar to stacking faults in crystals. Their contrasts depending only on the standard phase shift, they obey the rules established by Gevers [39], leading to the experimental determination of $\vec{r}_\parallel$. The contrasts are symmetrical in bright field (note the bright outer fringe, arrowed in Fig. 3(a)) and asymmetrical in dark field (arrows in Fig. 4(b)). Contrast analyses allow one to determine the corresponding displacement vector $\vec{r}_\parallel$. For the case of dislocations, when there is no phason dispersion, the dislocation Burgers vectors have no component in $\mathbf{E}_\perp$, and their contrast depends only on the scalar product $\vec{g}_\parallel \cdot \vec{b}_\parallel$. The out-of-contrast condition $\vec{g}_\parallel \cdot \vec{b}_\parallel = 0$ is observed simultaneously for the dislocation (except in the case of strong residual contrast, as in Section 4.1, see dislocations 1 and 1′ in Figs. 3(d) and 4(d)) and for the fault, and no weak extinction is possible. Although values of $\vec{g}_\parallel \cdot \vec{b}_\parallel$ are irrational by nature, they are

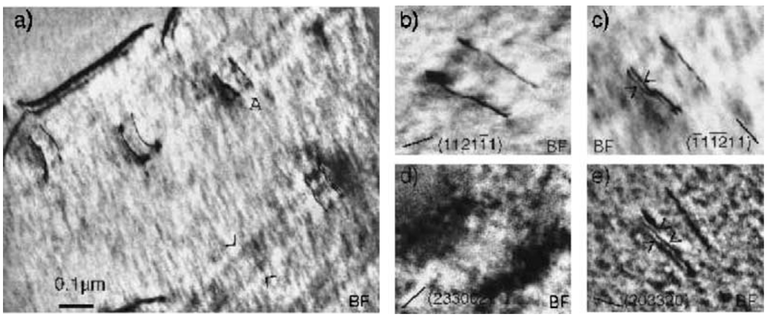

Fig. 3. Pure climb of dissociated 2-fold dislocations, in a sample deformed at 300 °C under a high confining pressure. Arrows in (a) underline the symmetrical phason fringe contrast in bright field conditions. Area A is shown in different conditions, with single contrasts in (b), a double contrast in (c), an extinction with some residual contrast in (d) and a triple contrast in (e).

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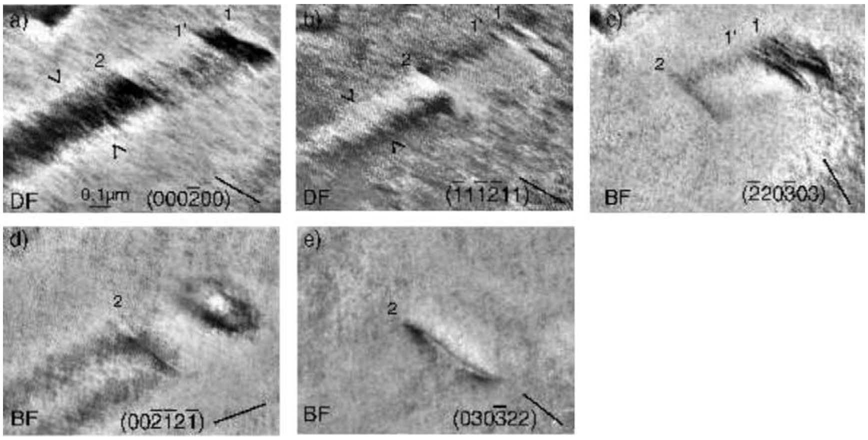

Fig. 4. Climb of imperfect 5-fold $(1-1')$ and 3-fold (2) dislocations in a 5-fold plane, in a sample deformed at 300 °C under a high pressure. (a) π-contrast of the APB between dislocations 1 and 1′ and in the wake of dislocation 2, imaged in dark field with a superstructure diffraction vector. (b) Normal asymmetrical contrast in dark field for a usual reflection, shown for comparison. (c) Double contrast of dislocations 1 and 1′. (d,e) Dislocations 1 and 1′ out of contrast with strong (d) and no (e) residual contrasts.

usually close to integer values, n, that correspond to contracts that are single ($n = 1$, Fig. 3(b), dislocations 1 and 1′ in Fig. 4(a) and (b)), and double ($n = 2$, Fig. 3(c), dislocations 1 and 1′ in Fig. 4(c), dislocation 2 in Fig. 4(e)). The same remark holds for large angle convergent beam electron diffraction patterns where the number of splittings is the closest integer to $\vec{g}_{\parallel} \cdot \vec{b}_{\parallel}$. The complete analysis shows that dislocations have 2-fold (Fig. 3), 5-fold (dislocations 1 and 1′ in Fig. 4) or 3-fold (dislocation 2 in Fig. 4) Burgers vectors, all out of the plane of motion This, again provides evidence for a climb process. In Fig. 4, the Burgers vector $[1/0, 0/1, 0/0]$ of dislocations 1 and 1′ is not issued from a translation of the 6-dim F-lattice but from a translation of the primitive P-lattice: dislocations 1 and 1′ are thus superpartial dislocations separated by an antiphase boundary (APB) ribbon. Fig. 4(a) shows that the APB viewed in dark field using a superstructure diffraction vector exhibits, as expected, a symmetrical π-type fringe contrast (see arrows).

4.3. In situ experiments

In situ observations have been carried out on samples heated at 700 °C, where the thermomechanical stresses are sufficient to induce dislocation motion. Fig. 5(a,b) shows two dislocations moving viscously in a 3-fold plane. They exhibit polygonal shapes along two 2-fold directions. A contrast analysis after cooling has shown that their Burgers vector has a component in the physical space along the 3-fold direction perpendicular to the plane of motion: this corresponds to a pure climb mechanism. The same phenomenon is observed on Fig.

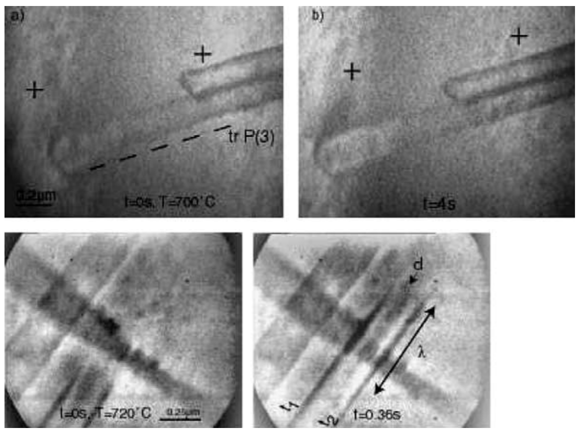

Fig. 5. In situ experiment showing: (a,b) 3-fold dislocations moving by pure climb at 700 °C; (c,d) a dislocation noted d, climbing in a 2-fold plane, and trailing over the length λ a rapidly dispersing phason fault at 720 °C.

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5(c,d) where a dislocation noted *d* climbs in a 2-fold plane. It appears fuzzy because of its high velocity. It trails two straight traces at the sample surfaces, noted t_1 and t_2, which slowly dissolve with time. A dark fringe is also visible between the traces, over the distance λ, to the dislocation. It is interpreted as a phason fault which disappears within 0.4 s by fast phason dispersion.

5. Conclusion

Although both glide and climb motions are theoretically possible in quasicrystals, geometrical and experimental evidences have been proposed here for privileging climb as the dominant motion mode in the plasticity of icosahedral quasicrystals. Glide motion should be considered as an appealing mechanism for inducing and propagating micro-cracks in the brittle regime of deformation. If climb is confirmed as the main motion mode, the phenomenological models so far proposed for the plastic deformation of quasicrystal would deserve profound physical revisions.

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