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Dislocations and mechanical properties of icosahedral quasicrystals

Dislocation et propriétés mécaniques des quasicristaux icosahédraux

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ABSTRACT

In this article we interpret the mechanical properties of icosahedral quasicrystals with the dislocation theory. After having defined the concept of dislocation in a periodic crystal, we extend this notion to quasicrystals in the 6-dimensional space. We show that perfect dislocations and imperfect dislocations trailing a phason fault can be defined and observed in transmission electron microscopy (TEM). In-situ straining TEM experiments at high temperature show that dislocations move solely by climb, a non-conservative motion-requiring diffusion. This behavior at variance with that of crystals which deform mainly by glide is explained by the atypical nature of the atomic structure of icosahedral quasicrystals.

RÉSUMÉ

Dans cet article, nous interprétons les propriétés mécaniques des quasicristaux icosahédriques par la théorie des dislocations. Après avoir défini le concept de dislocation dans les cristaux périodiques, nous étendons cette notion aux quasicristaux dans l'espace à 6 dimensions. Nous montrons que l'on peut définir et observer en microscopie électronique en transmission (MET) des dislocations parfaites et imparfaites traînant des fautes de phasons. Des observations en MET in situ à haute température montrent que les dislocations se déplacent uniquement par montée pure, un mouvement non conservatif requérant de la diffusion. Ce comportement, contraire à celui des cristaux qui se déforment principalement par glissement, est expliqué par la nature atypique de la structure atomique des quasicristaux icosahédraux.

1. Introduction

Quasicrystals are very brittle at low and medium temperatures, but start to be very ductile above about 70% of the absolute melting temperature. Such a behavior is at variance from that of most crystalline metals and alloys, which are plastic down to very low temperatures, even close to the zero absolute temperature. This difference is a priori not surprising, considering that crystals deform by the motion of perfect dislocations with Burgers vectors equal to the shortest distance of the periodic network, which cannot a priori exist in quasicrystals. Dislocations nevertheless do exist and account for the plastic

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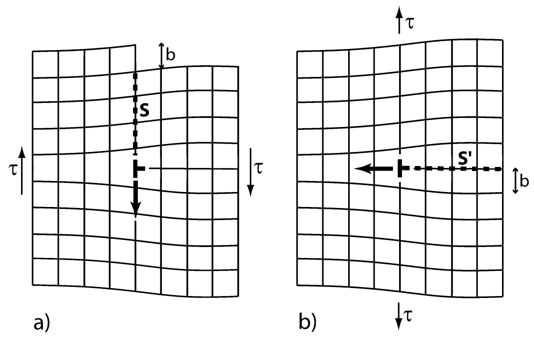

Fig. 1. Two Volterra processes, at the origin of the same perfect dislocation in a cubic crystal: a) along the surface S, by shear of amplitude b, b) along the surface S', by normal displacement of same amplitude b, and inserting new atoms to fill the gap.

deformation of quasicrystals, but their structure and their motion are different from those in crystals, in particular because this motion necessarily induces some disorder. It has long been considered that it is this disorder – and the short-range diffusion necessary to compensate it which is responsible for the difficult motion of dislocations at low temperature, and for the corresponding brittleness. This is however not the case, as shown in this article.

In the following paragraphs, we first introduce dislocations in crystals and quasicrystals. Then, we present experimental results showing that dislocations move by climb instead of glide (the main mode of motion in crystals), and that glide is forbidden or at least very difficult in quasicrystals. In the last part, we show that the climb motion is a direct consequence of the structure of quasicrystals, defined by the cut and projection procedure in the periodic high-dimensional lattice, and that it can account for the unusual mechanical properties.

2. Dislocations in crystals

Fig. 1 illustrates the creation and motion of dislocations in crystals. Perfect dislocations can be introduced in any crystal, by a Volterra process that does not depend on the cut plane. In Fig. 1a, an edge dislocation has been formed by cutting the crystal along the surface S, and shifting the two lips by the vector $\vec{b}$. If $\vec{b}$ is a translation vector of the lattice, the cut is perfectly healed, and the resulting dislocation is perfect. In Fig. 1b, the same perfect dislocation has been introduced by cutting the crystal along another surface S', and shifting the two lips by the same vector $\vec{b}$. Note that new atoms must be added along S' in this second case, in order to heal the cut plane and maintain the continuity of the crystal. Since the two results are identical, it results that perfect dislocations are defined by the displacement vector $\vec{b}$ alone (the Burgers vector), independently of the chosen cut plane. The result would of course be different if $\vec{b}$ were not a translation vector, because the cuts would not be healed, and the two (imperfect) dislocations would remain connected with two different faulted planes. A further motion of the dislocation in S, propagating a pure shear, is called glide, whereas a further motion in S', accompanied by the addition of new atoms originating from a long-range diffusion process, is called climb. Glide is usually observed in crystals deformed at low temperature, whereas climb (which requires thermally-activated long-range diffusion) is generally observed only above half the melting temperature.

3. Dislocations in icosahedral quasicrystals

Dislocations must be defined in the periodic 6-dimensional space from which the icosahedral structure is deduced, by cut and projection in the 3-dimensional physical space. In order to image this complex process, it is useful to consider the analogy of a 2-dimensional tiling obtained from the cut and projection of a 3-dimensional periodic lattice, presented in Fig. 2. Fig. 2a shows a 3-dimensional pile-up of cubes truncated by an irrational plane (close to, but different from a {111} plane). After projection in the cut plane and suppression of the shadow (Fig. 2b), the remaining cubes form an aperiodic 2-dimensional network consisting of three types of tiles. This figure also shows that the 2-dimensional tiling contains wavy bands of constant thickness (one is in white in Fig. 2b), also called worms, which are equivalent to the corrugated dense planes of the icosahedral structure, and which correspond to the emerging flat dense planes of the 3-dimensional periodic structure. Two types of Volterra processes similar to that shown in Fig. 1b can be hypothesized, yielding two types of dislocations:

- a Volterra process in the 2-dimensional aperodic network, by removing part of a band and connecting the two lips of the cut (Fig. 3a). This creates an imperfect dislocation with Burgers vector $\vec{b}_{\parallel}$, connected with a fault that can be easily visualized in Fig. 3b, where the relief of the cubes and the corresponding shadows have been restored. This fault corresponds to the phason planes trailed by imperfect dislocations in quasicrystals;
- a Volterra process in the 3-dimensional periodic network, by insertion (or removal) of a half extra plane (in black, in Fig. 4a), forming a 3-dimensional dislocation with Burgers vector $\vec{B}$. This first step is then completed by the same cut and projection as in Fig. 1, which results in a dislocation in the 2-dimensional tiling. This dislocation is perfect

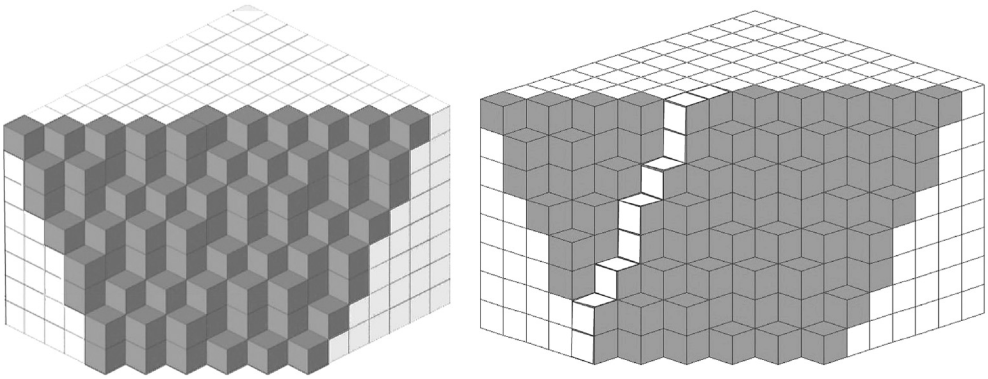

Fig. 2. Two-dimensional aperiodic tiling defined by cut and projection of a three-dimensional periodic cubic lattice. a) Truncated cubic lattice. b) Same structure as in a), after projection in the cut plane and suppression of the shadows. Note the wavy band, in bright, corresponding to the emergence of a dense plane. From [1].

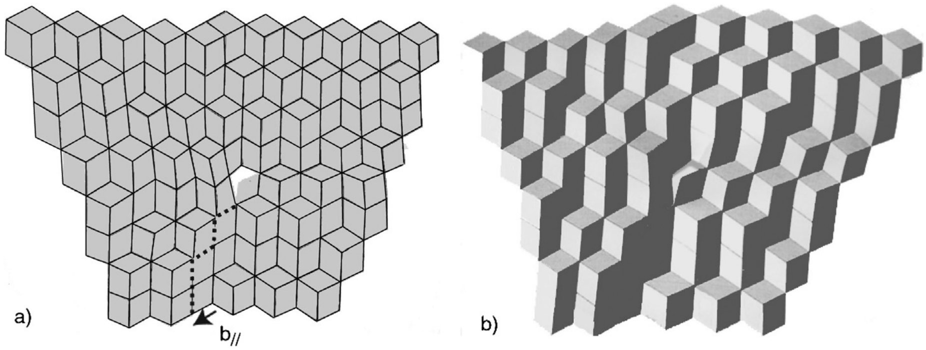

Fig. 3. Volterra process in the aperiodic tiling of Fig. 2, of displacement $\vec{b}_{\parallel}$ along the dotted line: a) without relief, and b) with the relief and corresponding shadows of the truncated pile-up of cubes. The relief shows that a fault remains along the cut, and that the dislocation is imperfect. From [1].

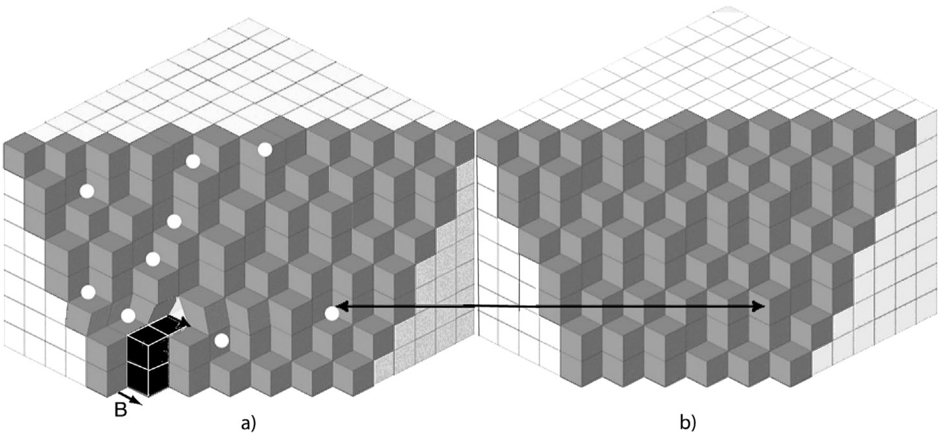

Fig. 4. Volterra process in the 3-dimensional pile-up of cubes of Fig. 2, generating a perfect dislocation with Burgers vector $\vec{B}$. After cut and projection, the aperiodic tiling in a) exhibits some differences with the original one in b), called phasons (white dots).

because there is no fault along the projection of the cut plane of the Volterra process. However, since the nodes of the 3-dimensional lattice have been displaced in the direction perpendicular to the projection plane, the latter does not intersect the very same cubes as before, which creates several tile inversions (missing or supplementary cubes, underlined by white dots) corresponding to a field of phasons. The dislocation is thus surrounded by an elastic field, with the corresponding Burgers vector $\vec{b}_{\parallel}$, and a phason field, defined by the displacement $\vec{b}_{\perp}$ normal to the projection plane. Both components of the Burgers vector $\vec{B} = \vec{b}_{\parallel} + \vec{b}_{\perp}$ are thus necessary to describe the dislocation in the 2-dimensional space. The total Burgers vector B, which has three components in the case of Fig. 3, has six components in the icosahedral structure.

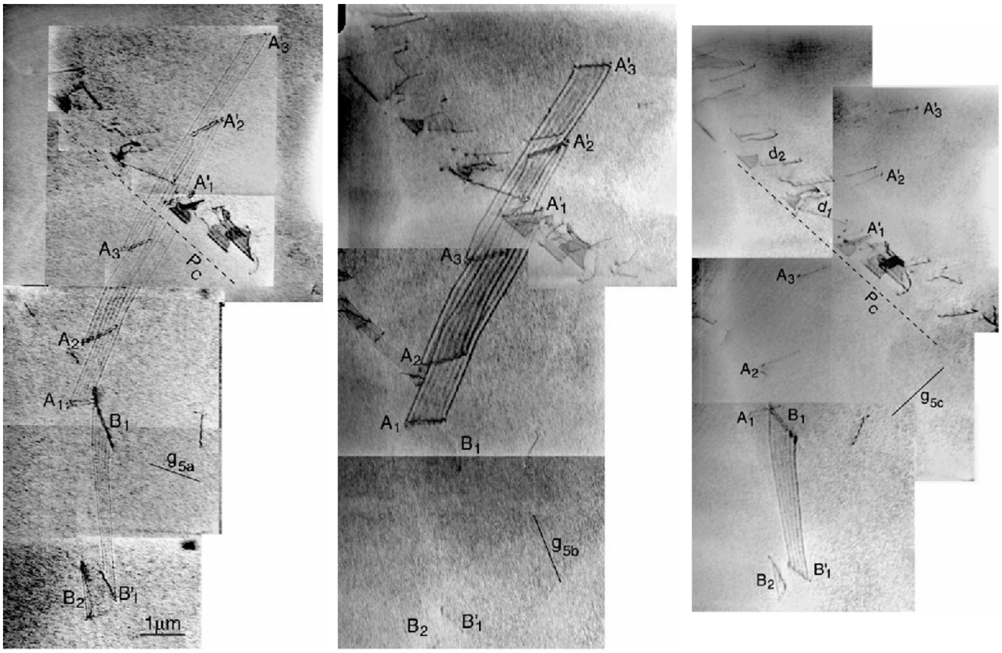

Fig. 5. Imperfect dislocations trailing phason faults, in as-grown AlPdMn. The different contrasts with the diffractions vectors $\vec{g}_{5a}$, $\vec{g}_{5b}$, and $\vec{g}_{5c}$ (all parallel to 5-fold directions of the reciprocal lattice) show that two types of dislocations (A_i and B_i) have moved by pure climb. From [26].

Both types of dislocations have been modeled by Gratias et al. [2], on the basis of the model of Quiquandon and Gratias [3]. They have been observed in the transmission electron microscope as reviewed in [4]. The experimental validation of the rules of contrast established in the 6-dimensional space in AlPdMn confirms the relevance of the cut and projection method:

- in the case of perfect dislocations, Wollgarten et al. [5,6] showed that the contrast depends on the scalar product $\vec{G} \cdot \vec{B}$, where $\vec{B}$ is the (six-dimensional) Burgers vector, and $\vec{G}$ is the (six-dimensional) diffraction vector. Of special interest is the weak extinction, for which $\vec{g}_{\parallel} \cdot \vec{b}_{\parallel} = \vec{g}_{\perp} \cdot \vec{b}_{\perp}$, i.e. the phase shift due to the elastic strain field is exactly compensated by the phase shift due to the chemical disorder, or phason field;
- in the case of imperfect dislocations, Mompiou et al. [7] showed that phason faults obey the same rules of contrast as stacking faults in crystals, depending on the irrational phase shift $\vec{g}_{\perp} \cdot \vec{b}_{\perp} = \vec{G} \cdot \vec{B} - \vec{g}_{\parallel} \cdot \vec{b}_{\parallel}$, where only $\vec{G} \cdot \vec{B}$ is the integer.

Perfect and imperfect dislocations have also been observed in the high-resolution mode [8–10] and by convergent-beam electron diffraction [11–14].

4. Moving dislocations

The first transmission electron microscope observations of AlPdMn deformed at high temperature (>750 °C) showed that the density of dislocations increases by two orders of magnitude with respect to the as-grown material [15]. Since these dislocations are perfect and form an isotropic network, it was however impossible to determine their plane of motion. The first in situ experiments showed dislocations moving viscously in well-defined planes [16], but here again it was not possible to determine simultaneously the Burgers vector and the plane of motion. Under such conditions, dislocations were assumed to move by glide, i.e. in planes containing the component $\vec{b}_{\parallel}$ of their Burgers vector. Several models have been subsequently proposed to account for the high brittle-to-ductile transition temperature, involving Peierls–Nabarro friction forces [17–20], or cutting through highly ordered pseudo-Mackay clusters [21–23].

Contrary to this assumption, the first complete analyses in AlPdMn showed that imperfect dislocations trailing phason faults are in planes perpendicular to their Burgers vector $\vec{b}_{\parallel}$ [24,25], in agreement with a pure climb process (Fig. 5). Later on, in situ observations showed that perfect dislocations also move by pure climb in planes perpendicular to the component $\vec{b}_{\parallel}$ of their Burgers vector (Fig. 6).

In situ observations also showed that there is no fundamental difference between the climb motion of imperfect and perfect dislocations, except for the higher stress necessary to compensate the lower temperature, in the case of imperfect ones. Indeed, consider the motion of a perfect dislocation, under an applied stress (Fig. 7a): since the stress acts on the sole component $\vec{b}_{\parallel}$, the perfect dislocation tends to dissociate into a moving component of Burgers vector $\vec{b}_{\parallel}$, trailing a

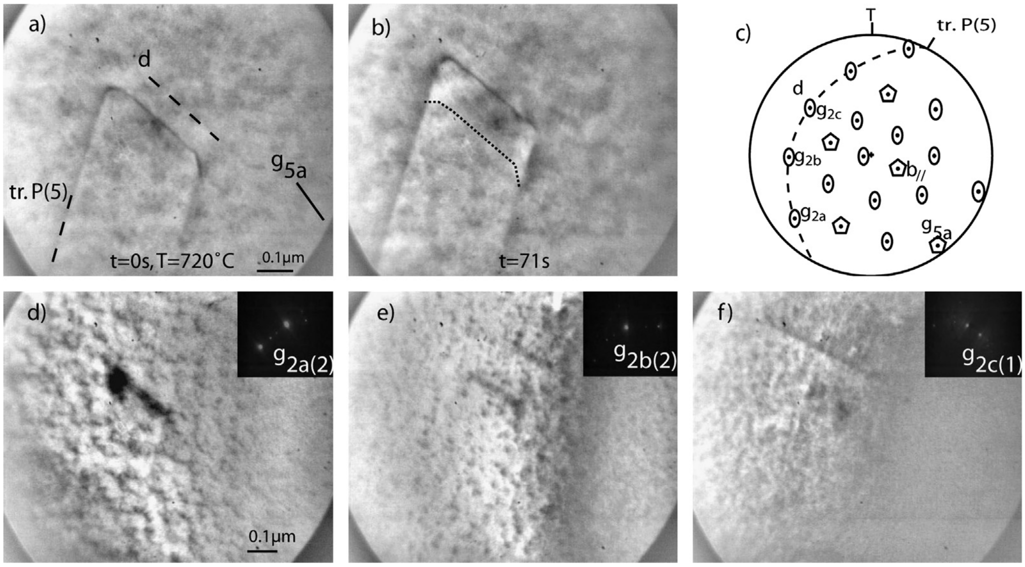

Fig. 6. Perfect dislocation moving in a 5-fold plane of AlPdMn at 720 °C, and contrast analysis showing pure climb motion. a),b) Dislocation motion. c) Stereographic projection showing the dislocation direction $\vec{d}$, the Burgers vector component in the physical space, $\vec{b}_{\parallel}$, the different g-vectors, and the trace of motion at the sample surface (tr.P(5)) corresponding to the 5-fold plane perpendicular to $\vec{b}_{\parallel}$ (in dotted line). d)–f) Out-of-contrast conditions, for Burgers vector determination. From [27].

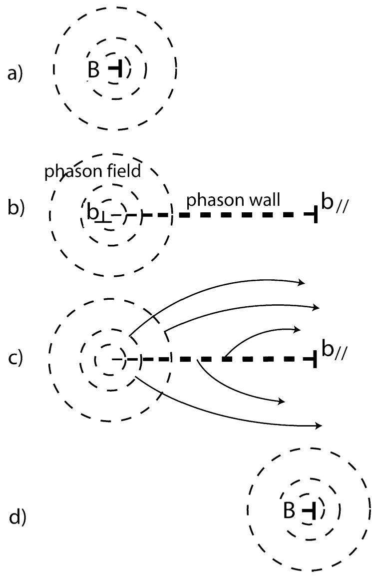

Fig. 7. Schematic description of the motion of a perfect dislocation under stress. a) Initial state, where equi-phason density lines are schematized by dotted circles. b) Motion of the component $\vec{b}_{\parallel}$, and creation of a phason fault. c) Dispersion of the phason fault, when the temperature is high enough. d) Restoration of the initial perfect dislocation after motion. The two intermediate steps b) and c) correspond to the dynamic dissociation of $\vec{B}$ into $\vec{b}_{\parallel}$ and $\vec{b}_{\perp}$|.

phason fault, and a sessile component of Burgers vector $\vec{b}_{\perp}$, which is the limit of the phason fault at the initial dislocation place (Fig. 7b). The phason fault is however unstable at high temperature and tends to spread out by diffusion of individual phasons, as schematized in Fig. 7c. If now the stress is released, the component $\vec{b}_{\parallel}$ stops moving and is rapidly surrounded by the diffusing phasons, until the perfect dislocation structure is restored (Fig. 7c, d). Under such conditions, the different mechanisms observed just correspond to different kinetics of phason diffusion:

– very slow diffusion at low temperature, leading to imperfect dislocations trailing long stable phason faults;
– faster diffusion at intermediate temperature, leading to imperfect dislocations trailing rapidly vanishing phason faults (Fig. 8), namely to moving dissociated dislocations like in Fig. 7b;

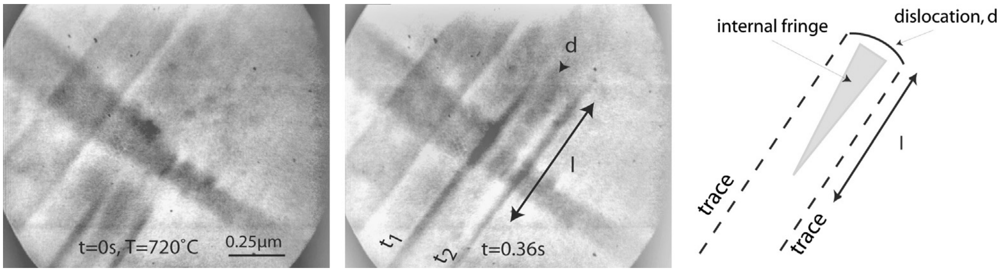

Fig. 8. Imperfect dislocation trailing a rapidly vanishing phason wall of length l, in a 2-fold plane. The dynamic dissociation of width l corresponds to Fig. 7b–c. In situ experiment in Al–Pd–Mn at 720 °C, from [27].

– very fast diffusion at high temperature, corresponding to the quasi-simultaneous motion of the two components $\vec{b}_{\parallel}$ and $\vec{b}_{\perp}$, namely to moving perfect (non-dissociated) dislocations.

In the latter case, and since the applied stress acts on the component $\vec{b}_{\parallel}$ only, the dislocation motion is still controlled by the climb motion of this component, even if the width of the phason fault ribbon (the dissociation width) tends to very small values. In other words, and contrary to the first hypotheses concerning the motion of dislocations in quasicrystals, the plastic deformation is not controlled by the diffusion of phasons, but by the highly thermally activated climb motion of the elastic part of dislocations with Burgers vectors $\vec{b}_{\parallel}$. The production of phason faults at all temperatures is nevertheless at the origin of a back stress which must be added to the climb stress. However, since the surface energy of phason faults, deduced from the equilibrium width of dissociated dislocations at low temperature is fairly low (of the order of 24 mJ/m^2 according to [25]), the corresponding back stress is also low, of the order of 30 MPa, i.e. quite negligible at medium temperature. The climb stress is accordingly the main part of the total deformation stress.

5. Climb versus glide

Microscopic observations in TEM have shown that the relative ease of the two modes of dislocation motion, glide versus climb, is reversed in quasicrystals with respect to crystals. Indeed, glide (which corresponds to the propagation of a shear displacement according to Fig. 1a) is the easiest mode in crystals, and the only one taking place at low temperature in ordinary metals and alloys. Still in crystals, climb (which corresponds to the precipitation or dissolution of a dense plane according to Fig. 1b) starts only above half the absolute melting temperature, where it is more and more mixed with glide. On the contrary, only climb can be observed in quasicrystals. As a result of this difference, the kinetics of formation and annihilation of edge dipoles (pairs of edge dislocations with opposite Burgers vectors) are very different in crystals and quasicrystals. In crystals, edge dipoles are formed by fast glide, and annihilated by slow climb, whereas in quasicrystals they are formed by fast climb, and possibly annihilated by very slow glide. Fig. 9 is an example of the latter situation, in AlPdMn where two dislocations move in opposite directions by pure climb, and form a dipole that remains stable during more than one hour at 750 °C, just because their annihilation would require highly difficult glide. The highly difficult glide of dislocations in AlPdMn is directly related to the geometry of the icosahedral quasicrystalline structure. Indeed, the dense planes, which result from the emergence of the flat dense planes of the periodic high-dimensional structure, are very corrugated (as the wavy white band in Fig. 1), in such a way that any shear along these planes is necessarily difficult. Fig. 10 shows that the shear of a Penrose tiling along a horizontal worm (equivalent to a dense plane) creates heavily distorted zones that cannot be retiled with available tiles. The corresponding fault plane (the phason fault) has a very high surface energy, of the order of 1 J/m^2 [29], which induces a huge back stress on gliding dislocations. On the contrary, a displacement perpendicular to the same worm, corresponding to the removal or duplication of a complete corrugated gray band of constant thickness, does not create the same disorder. The latter displacement of course induces some violations of the tiling rules, corresponding to the formation of a phason fault, but costing much less energy (only 24 mJ/m^2 in AlPdMn according to our measurements). The demonstration that the only dislocation motion that keeps the internal tiling coherent (with no empty space nor overlap in the trace of motion) is obtained for pure edge dislocations moving by pure climb has been made by Gratias et al. [2]. Although pure climb requires atomic displacements over long distances by long-range diffusion, it is the easiest mode of deformation on the topological point of view in quasicrystals.

All the mechanical properties of quasicrystals can now be explained on the basis of the pure climb motion of dislocations [30]. The low-temperature brittleness is directly related to the impossibility of glide. Since climb is highly thermally activated, plastic deformation is possible only at high temperature, under normal deformation stresses, or at moderate temperature, under very high deformation stresses accessible under indentation, or under a very high confining pressure. In this respect, quasicrystals can be compared to covalent crystals like silicon, where glide is highly thermally activated and thus very difficult at low temperature. Besides, it has been shown that glide in semiconductors and climb obey similar mobility equations, although the parameters involved have a different physical meaning, related to the cutting of covalent bonds in semiconductors, and to the diffusion of atoms in quasicrystals.

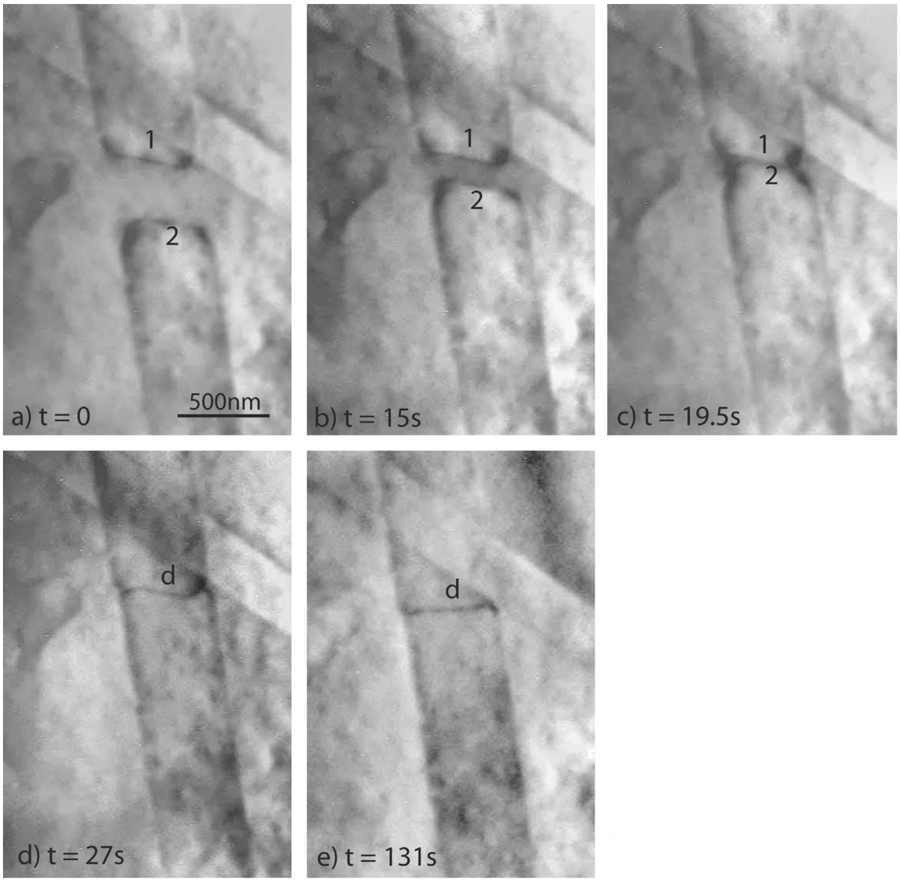

Fig. 9. Formation of a stable dislocation dipole d, by climb of opposite dislocations in closely parallel planes. The dipole cannot annihilate because this would require highly difficult glide. From [28].

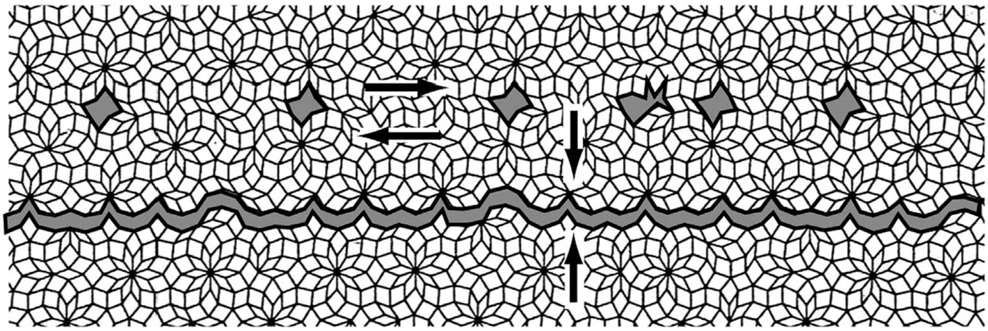

Fig. 10. Comparison between the topological defects introduced by glide (top, from Mikulla et al. [29]) and climb (bottom), in a Penrose tiling. Glide generates zones that cannot be retiled, whereas climb just needs annihilation or duplication of worms.

6. Conclusions

In conclusion, the mechanical properties of quasicrystals are now almost completely elucidated. They do not involve any new deformation mechanism, and can be entirely described by the pure climb motion of dislocations trailing phason faults. This difference with respect to crystals is a direct consequence of the high corrugation of the dense planes, which itself results directly from the cut and projection procedure describing quasicrystals. This, and the contrast of dislocations in TEM, are among the most relevant validations of the description of quasicrystals in a high-dimensional space.

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