Materials Science and Engineering A 387–389 (2004) 89–92

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Dislocation climb in an Al–Pd–Mn quasicrystal deformed at low temperature

F. Mompiou*, J. Crestou, D. Caillard

CEMES-CNRS, 29 rue J. Marvig BP 4347, 31055 Toulouse cedex, France

Received 26 August 2003; received in revised form 15 December 2003

Abstract

Dislocations and phason faults have been imaged in a transmission electron microscope in an icosahedral Al–Pd–Mn quasicrystal deformed at 300 °C. The contrast of these dislocations has been studied. The analysis of Burgers vectors indicates that their motion takes place by climb.

Keywords: Quasicrystal; Phason fault; Climb

1. Introduction

Quasicrystals can be defined as a structure with orientational order and no translational symmetry [1]. However, although they lack periodicity, icosahedral quasicrystal such as Al–Pd–Mn, can be described in a six-dimensional ordered face-centered hypercubic lattice [2] composed by the physical subspace ($E_{\parallel}$) and the perpendicular subspace ($E_{\perp}$). Dislocations can, formally, be introduced by a Volterra process either in the 6D space or in the 3D physical space. In the 6D space, the two lips of the cut can be perfectly glued, thanks to the periodicity of the structure. This process yields a perfect dislocation after projection into the physical space. The corresponding Burgers vector, $\boldsymbol{B}$, is a translation vector of the 6D lattice with a phonon component $\boldsymbol{b}_{\parallel}$ in physical space (elastic field) and a phason component $\boldsymbol{b}_{\perp}$ in perpendicular space. The latter corresponds to a cloud of point defects (phasons) that compensates for the lack of translational symmetry. If the Volterra process is performed directly in the physical space, the lips of the cut cannot be glued perfectly due to the lack of periodicity. Fig. 1(a) shows the Volterra process in a non-periodic 2D tiling. Matching rules between adjacent tiles have been represented in a portion of the tiling (arrows). An edge dislocation can be obtained by removing a half "quasi-plane" in the tiling and joining the two lips of the cut. An elastic field is then produced around the dislocation core (A). Although the topology of the tiling is preserved during this process, several mismatches are introduced in the plane of the cut as opposite arrows bounding the lips of the cut indicate. Fig. 1(b) is the representation of such an imperfect dislocation. The dislocation is characterized by its Burgers vector $\boldsymbol{b}_{\parallel}$. It trails a so-called "phason fault" which can be seen as a kind of stacking fault with a displacement vector $\boldsymbol{R} = \boldsymbol{b}_{\parallel}$ or $-\boldsymbol{b}_{\perp}$ (note that both quantities are equivalent since they differ by $\boldsymbol{B}$, a translation vector of the periodic structure). The fault can be considered as the condensation of the individual phasons distributed around the perfect dislocation described above (for further details see [3,4]). Conversely, the dispersion of individual phasons around an imperfect dislocation leads to a perfect dislocation. This process is thermally activated and is called "retiling", or phason dispersion.

As in ordinary crystals, dislocations move and multiply under local and external stress fields [5]. Their mode of motion is however still a subject of controversy. Previous studies concluded on a glide mechanism controlled by crossing either clusters [6] or Peierls valleys [7]. However, evidence of climb (i.e. $\boldsymbol{b}_{\parallel}$ out of the plane of motion) has also been found in as-grown samples [4,8,9]. In these new experiments, samples have been deformed in compression under a high confining pressure which allows plastic deformation at temperatures as low as 300 °C. Consequently, no retiling is expected, and as the planes of motion can be identified with the phason faults planes, they can be determined

* Corresponding author. Tel. +33 562 257 872; fax: +33 562 257 999.
E-mail address: mompiou@cemes.fr (F. Mompiou).

0921-5093/$ – see front matter
doi:10.1016/j.msea.2004.01.076

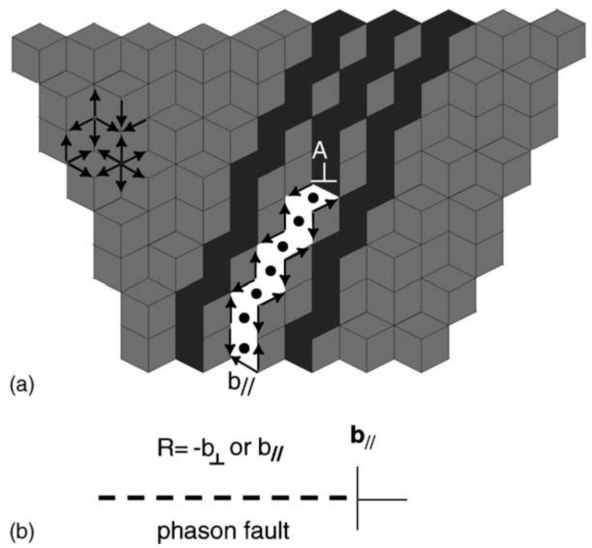

Fig. 1. (a) Representation of the Volterra process in a 2D non-periodic tiling partially decorated by arrows indicating the matching rules. (b) An imperfect edge dislocation (at A) and a phason fault in the cut plane are formed as schematized.

unambiguously. Then, provided the Burgers vectors can be deduced from TEM contrast experiments, climb can easily be distinguished from glide.

2. Experimental details

Specimens for TEM investigations were cut from a sample deformed of a few percent at 300 °C in compression under a high confining hydrostatic pressure (5–7 GPa). They were ground and subsequently thinned by conventional ion milling under cooling. Other samples milled by a precision ion polishing system did not contain any phason faults. In fact, this technique can induce very high local heating, which can introduce substantial phason fault retiling.

3. Contrasts of dislocations and phason faults in TEM

Extinction rules have been established for perfect dislocations, beyond the framework of the kinematical approximation, considering the displacement field in the six-dimensional space [10]. They have been checked in i-Al–Pd–Mn [11] and extended to the case of multiple contrast and residual contrast [12]. In the case of imperfect dislocations, we have concluded that the same rules of contrast can be used considering only phase shifts in physical space. We have also specified the contrast behaviour of phasons faults. This section summarizes all the different rules, with reference to dislocations that will be discussed more extensively in Section 4.

The phason fault behaves exactly as a stacking fault in a crystal. Their contrast obeys Gevers' rules [13] based on the scalar product $\boldsymbol{G}{\cdot}\boldsymbol{R}$, where $\boldsymbol{R}$ is the displacement vector of the fault. Fig. 2(a) shows two identical dislocations (d_1 and d_2) trailing a phason fault. Note the symmetrical fringe contrast in bright field (v-shaped markers indicate the bright external fringes). According to Gevers, the nature of the outer fringe allows one to determine the sign of $\boldsymbol{R}$ for a given diffraction vector. For an imperfect dislocation, the invisibility criterion $\mathbf{G}.\mathbf{B} = 0$ reduces to $\boldsymbol{g}_{\parallel} \cdot \boldsymbol{b}_{\parallel} = 0$ since $\boldsymbol{b}_{\perp} = 0$. Fig. 2(b) and (c) show extinction conditions for the two dislocations with a rather strong residual contrast which can be interpreted by a high value of $\boldsymbol{g}_{\parallel}(\boldsymbol{b}_{\parallel} \times \mathbf{u})$, where $\mathbf{u}$ is the line direction. Note that the phason fault is clearly out of constrast too. A double contrast condition is realized when $\boldsymbol{G}{\cdot}\boldsymbol{B} = 2$ which reduces to $\boldsymbol{g}_{\parallel} \cdot \boldsymbol{b}_{\parallel} \approx 2$ for an imperfect dislocation because $\boldsymbol{g}_{\perp}{\cdot}\boldsymbol{b}_{\perp}$ is irrationnal and usually small (Fig. 2(d)). A case of special interest arises for perfect dislocations when the phase shift introduced by the phason field compensates exactly that of the elastic field, i.e. $\boldsymbol{g}_{\parallel} \cdot \boldsymbol{b}_{\parallel} = -\boldsymbol{g}_{\perp} \cdot \boldsymbol{b}_{\perp}$. This leads to a "weak extinction". This condition cannot be met for imperfect dislocations where $\boldsymbol{b}_{\perp} = 0$. However, in that case the contrast of the dislocation is weak because $\boldsymbol{g}_{\parallel} \cdot \boldsymbol{b}_{\parallel} \ll 1$. This is called a "pseudo-weak" extinction, and the dislocation appears just as the limits of the phason fault fringe pattern as in the case of Shockley partials bounding a stacking fault in a crystal under the condition of $\boldsymbol{g}{\cdot}\boldsymbol{b}_{\mathbf{p}} = \pm 1/3$. Fig. 3 shows this condition for another dislocation. All these conditions allow us to determine the Burgers vectors, unambiguously.

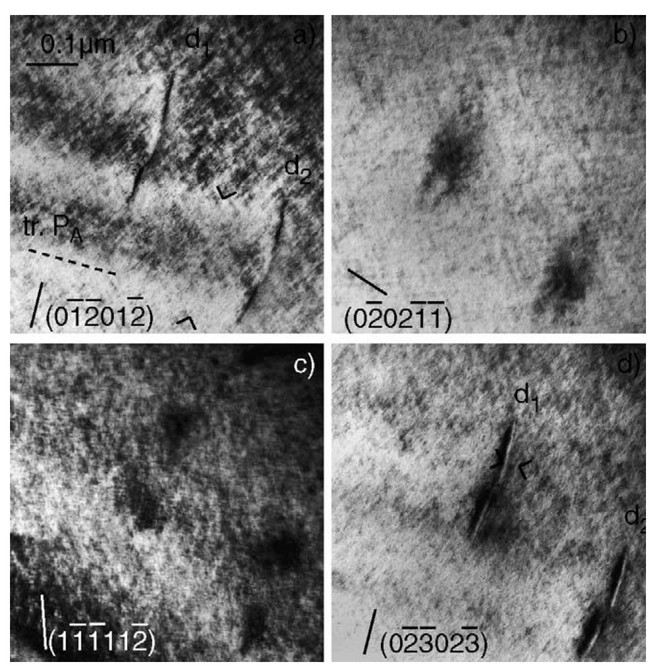

Fig. 2. Bright-field TEM images of imperfect dislocations. (a) Single contrast condition with the symmetrical fringe pattern of the phason fault. (b) and (c) Extinction conditions with strong residual contrast. (d) Double contrast condition.

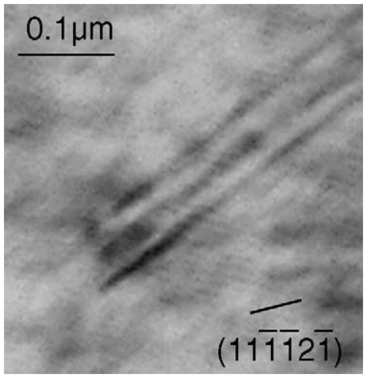

Fig. 3. TEM image of an imperfect dislocation in a “pseudo-weak” extinction condition.

4. Main results and discussion

Several dislocation families have been found. All the dislocations exhibit phason faults in their wake, as described Fig. 1(b).

The dislocations shown in Fig. 2 have moved in the (1/0, 1/1, 0/1) two-fold plane inclined 31.71° from the compression axis as the trace direction of the phason fault plane (tr. P_A) and the variation of its width as a function of the tilt angle indicate. The two extinction conditions (Fig. 2(b) and (c)) show that the Burgers vector is normal to the plane of motion. The dislocations have, accordingly, moved by climb. With the single and double contrast conditions (Fig. 2(a) and (d), respectively) we find that $\boldsymbol{b}_{A\parallel} = [\bar{1}/1, 0/1, 1/0]$ of length 0.479 nm. The two main dislocation systems containing the highest dislocation densities are described below. Dislocations of the first system are shown in Fig. 4(a). They have moved in the five-fold planes perpendicular to the compression axis. Several dislocations move in the same plane: two paired dislocations are usually found at the front, followed by one or more individual ones (in the inset). The contrast analysis leads to the following conclusions:

- Paired dislocations are superpartials dislocations (note that the 6D structure is ordered with a superstructure). They are separated by an antiphase boundary ribbon. Their Burgers vector is perpendicular to the plane of motion;
- others dislocations have Burgers vectors oriented along two-fold or three-fold axis also out of the plane of motion;
- the phason fault has a “vacancy” character.

Dislocations of the second system (Fig. 4(b)) have moved in planes parallel to the compression axis and the same analysis as above leads to the following conclusions:

- they have two-fold Burgers vectors perpendicular to the plane of motion.
- the phason fault has an “interstitial” character.

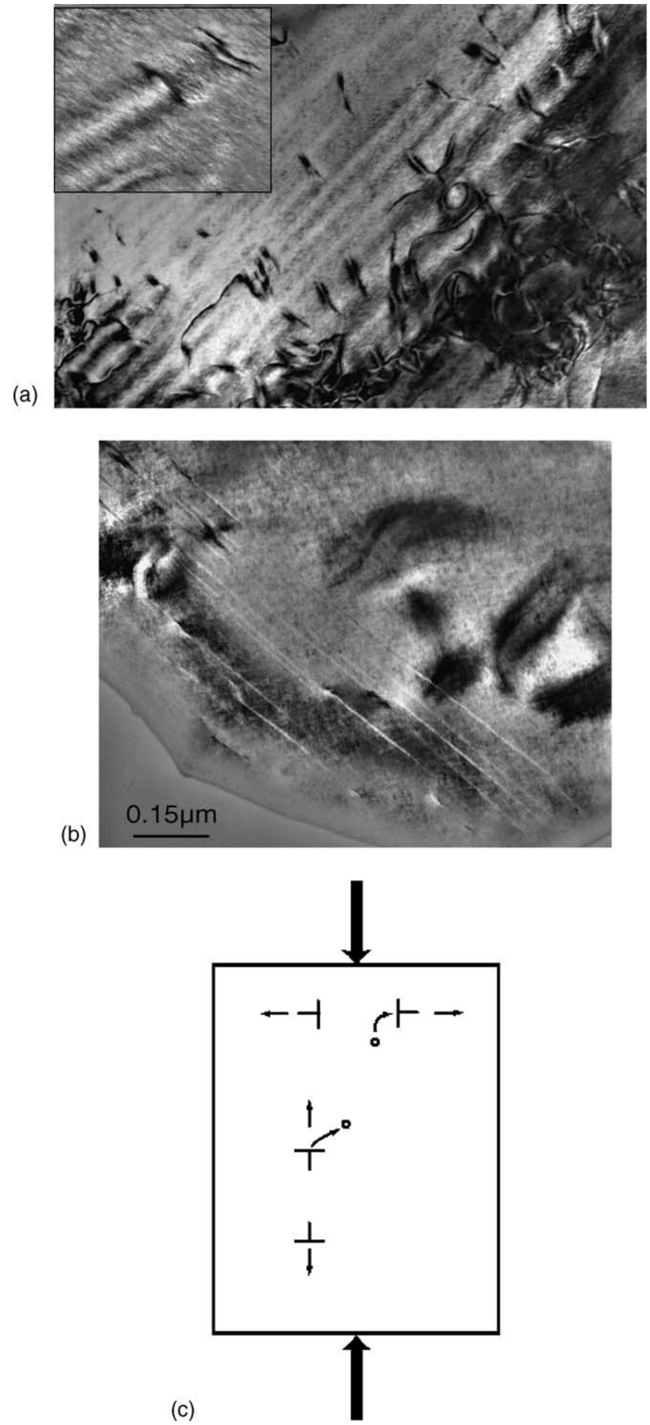

Fig. 4. (a) Motion of dislocations of the first and second system (b) seen edge-on. Note the strong residual contrast of the dislocations of the first type in (b). (c) The cooperative climb motion with exchange of matter between the two systems is described schematically.

All the observed dislocations have moved by a climb mechanism. In-situ experiments in a TEM at higher temperatures [14] confirm these conclusions. As described in Fig. 4c, the two main systems are related to each other by a concomitant exchange of matter, the second providing vacancies to the first one.

5. Conclusion

We have described the contrast of non-retiled dislocations in i-Al–Pd–Mn deformed in compression at 300 °C. All the dislocations have moved by climb. Although dislocation motion by glide is theorically possible, climb appears to be the dominant mode of motion in icosahedral quasicrystals.

References

[1] D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, Phys. Rev. Lett. 53 (1984) 1951.
[2] M. Boudart, M. De Boissieu, Ch. Janot, G. Heger, C. Beeli, H.U. Nissen, H. Vincent, R. Ibberson, M. Audier, J.M. Dubois, J. Phys. Cond. Mat. 50 (1992) 10149.
[3] D. Caillard, F. Mompiou, L. Bresson, D. Gratias, Scripta. Mater. 49 (2003) 11.
[4] D. Caillard, G. Vanderschaeve, L. Bresson, D. Gratias, Phil. Mag. A 80 (2000) 237.
[5] M. Wollgarten, M. Bartsch, U. Messerschmidt, M. Feuerbacher, R. Rosenfeld, M. Beyss, K. Urban, Phil. Mag. Lett. 71 (1995) 99.
[6] M. Feuerbacher, C. Metzmacher, M. Wollgarten, B. Baufeld, M. Bartsch, U. Messerschmidt, K. Urban, Mater. Sci. Eng. A 233 (1997) 103.
[7] S. Takeuchi, R. Tamura, E. Kabutoya, Phil. Mag. A 82 (2002) 379.
[8] D. Caillard, C. Roucau, L. Bresson, D. Gratias, Acta. Mater. 50 (2002) 4499.
[9] D. Caillard, J.-P. Morniroli, G. Vanderschaeve, L. Bresson, D. Gratias, Eur. Phys. J. AP 20 (2002) 3.
[10] M. Wolgarten, D. Gratias, Z. Zhang, K. Urban, Phil. Mag. A 64 (1991) 819.
[11] M. Wollgarten, Z. Zhang, K. Urban, Phil. Mag. Lett 65 (1992) 1.
[12] F. Mompiou, L. Bresson, P. Cordier, D. Caillard, Phil. Mag. 83 (2003) 3133.
[13] R. Gevers, in: B. Jouffrey (Ed.), Méthodes et Techniques Nouvelles d'Observation en Métallurgie Physique, SFME, Paris, 1972, pp. 155.
[14] F. Mompiou, M. Feuerbacher, D. Caillard, Phil. Mag., in press.