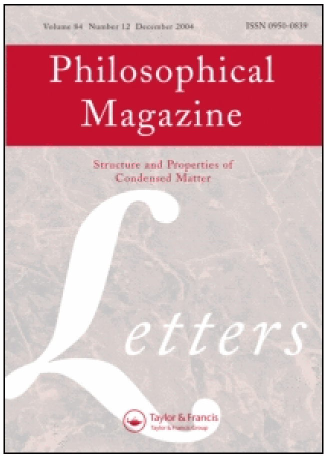

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Phason–phonon-assisted epitaxy at icosahedral–decagonal interfaces in Al–Pd–Mn quasicrystals

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ABSTRACT

Platelets of the Al–Pd–Mn decagonal phase have been observed to grow in epitaxy on the icosahedral modification of the same system. A resulting strain field in the icosahedral phase has been characterized using high-resolution electron microscopy. It appears that one fivefold axis is preserved, in coincidence with the tenfold axis of the decagonal phase. In the particular case of a thin icosahedral-phase domain squeezed in between two decagonal-phase platelets, the strain field can be qualitatively analysed in terms of combined phason–phonon strain fields.

§ 1. INTRODUCTION

Precipitate–matrix interfaces, as observed in periodic alloy systems, have been extensively investigated (e.g. see review articles by Ecob (1985) and Aaronson *et al.* (1990)). Geometrical theories such as the O-lattice model (Bollmann 1967) or crystallographic invariance line determination (Dahmen 1982) are generally associated with energetic considerations in order to interpret why interface structures are coherent, semicoherent (with interfacial dislocation lattices) or incoherent (with interfacial ledge structures).

The particular case of interfaces in quasicrystalline materials, or at periodic–quasiperiodic boundaries, has opened a new field of interest. However, it is still questionable whether the 'periodic models' could be extended to quasiperiodic phases within their hyperspace description.

In the present paper, some properties of quasicrystal interfaces are reported, as deduced from icosahedral–decagonal phase intergrowth in the Al–Pd–Mn system (de Boissieu *et al.* 1992a). This system is a good candidate for an accurate investigation of the strain field that should result from forced epitaxy. Both decagonal and icosahedral Al–Pd–Mn phases are actually known to be perfect quasicrystals and their interfaces can be perfectly planar and structurally coherent. This may facilitate the analyses of high-resolution electron microscopy (HREM) images and their understanding in terms of phason and phonon strains on the basis of published models (Lubensky *et al.* 1986, Ishii 1989, Qiu and Jaric 1989). This is going to be demonstrated further in the forthcoming sections of the paper.

§ 2. SAMPLES AND EXPERIMENTAL RESULTS

Centimetre-sized single grains of the Al–Pd–Mn icosahedral phase have been obtained (de Boissieu *et al.* 1992) via a classical two-step procedure: induction melting

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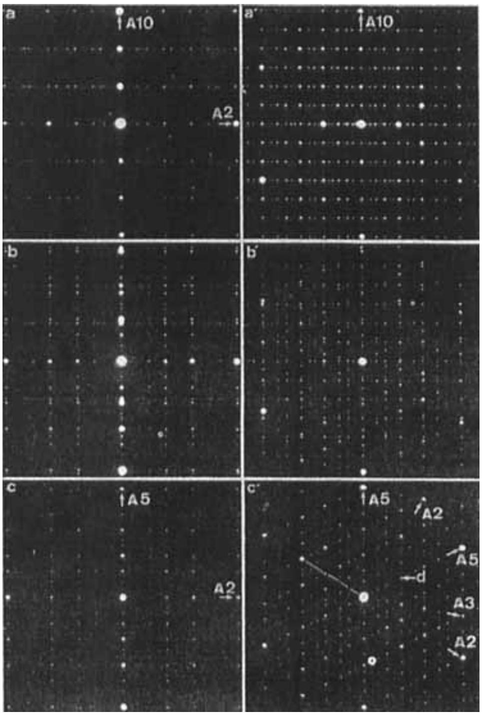
of the elements in a cold crucible followed by a standard Bridgman crystal growth in an alumina crucible. Such large single grains have been used previously for X-ray and neutron diffraction measurements and structural studies (Boudard *et al.* 1991).

Depending on the actual composition and annealing treatments, scanning electron microscopy observations of polished sections have occasionally shown large platelets of a decagonal phase (de Boissieu *et al.* 1992b). An electron probe microanalysis has demonstrated a compositional misfit between the icosahedral ($\mathrm{Al}_{68\cdot3}\mathrm{Pd}_{23}\mathrm{Mn}_{8\cdot6}$) and the decagonal ($\mathrm{Al}_{67\cdot5}\mathrm{Pd}_{14\cdot6}\mathrm{Mn}_{17\cdot9}$) phases. Transmission electron microscopy (TEM) and electron diffraction have allowed the structural properties of the decagonal platelets to be specified (Audier, de Boissieu and Guyot 1992). This structure appears to be closely related to that of an isomorphous Al–Pd–Mn compound of the $\mathrm{Al}_{13}\mathrm{Fe}_4$ monoclinic phase (Black 1955). The parameters are $a = 4\cdot1(\pm 0\cdot05)\tau^n$ Å (with n integer and τ the golden mean) and $c = 12\cdot43$ Å. The icosahedral phase has a lattice parameter of $6\cdot451\tau^n$ Å in its six-dimensional cubic image (de Boissieu *et al.* 1992a), which projects a distance of $4\cdot08$ Å $(= 6\cdot451\cos(\pi/2 - 63\cdot43°)/2^{1/2})$ into a fivefold zone axis of the physical space. Within experimental accuracy, the quasilattice misfits for epitaxial relationship between icosahedral and decagonal phases appear to be reasonably weak.

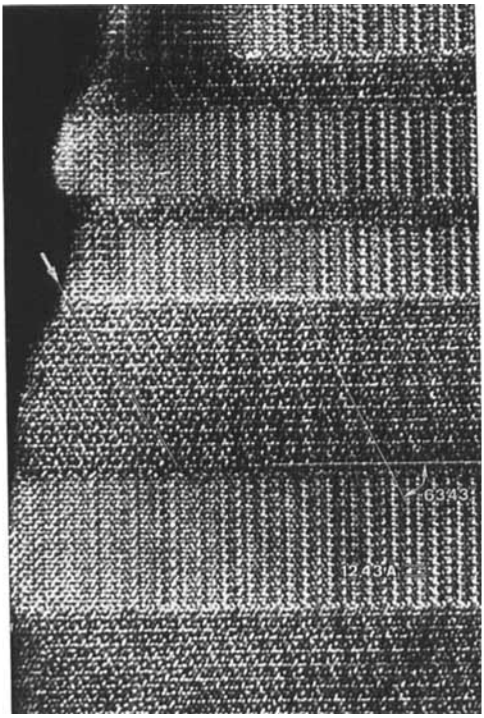
Electron diffraction patterns (fig. 1) and the corresponding HREM micrographs (fig. 2) have clearly demonstrated epitaxy of the two phases with a coherent interface

Fig. 1



Electron diffraction patterns corresponding to a single icosahedral–decagonal interface: the two columns of patterns are related by a rotation of 18° about the vertical tenfold axis of symmetry of the decagonal phase (or the parallel icosahedral fivefold axis). In each column the patterns correspond successively to (*a*), (*a*′) the decagonal phase, (*b*), (*b*′) the decagonal–icosahedral interface and (*c*), (*c*′) the icosahedral phase. The arrowed reflection d in the pattern (*c*′) corresponds to a distance of $1\cdot1142\ \text{Å}^{-1}$ from the centre.

Fig. 2



High-resolution dark-field electron micrograph showing several sandwiches of icosahedral phase between lamellae precipitates of decagonal phase; their crystallographic orientations correspond to those shown in figs. 1 (*a*′), (*b*′) and (*c*′). The 63·43° angle between traces of the fivefold planes is indicated, as well as the periodicity of 12·43 Å measured along the tenfold axis of the decagonal phase. This dark-field micrograph has been obtained by selecting a set of reflections along the tenfold axis.

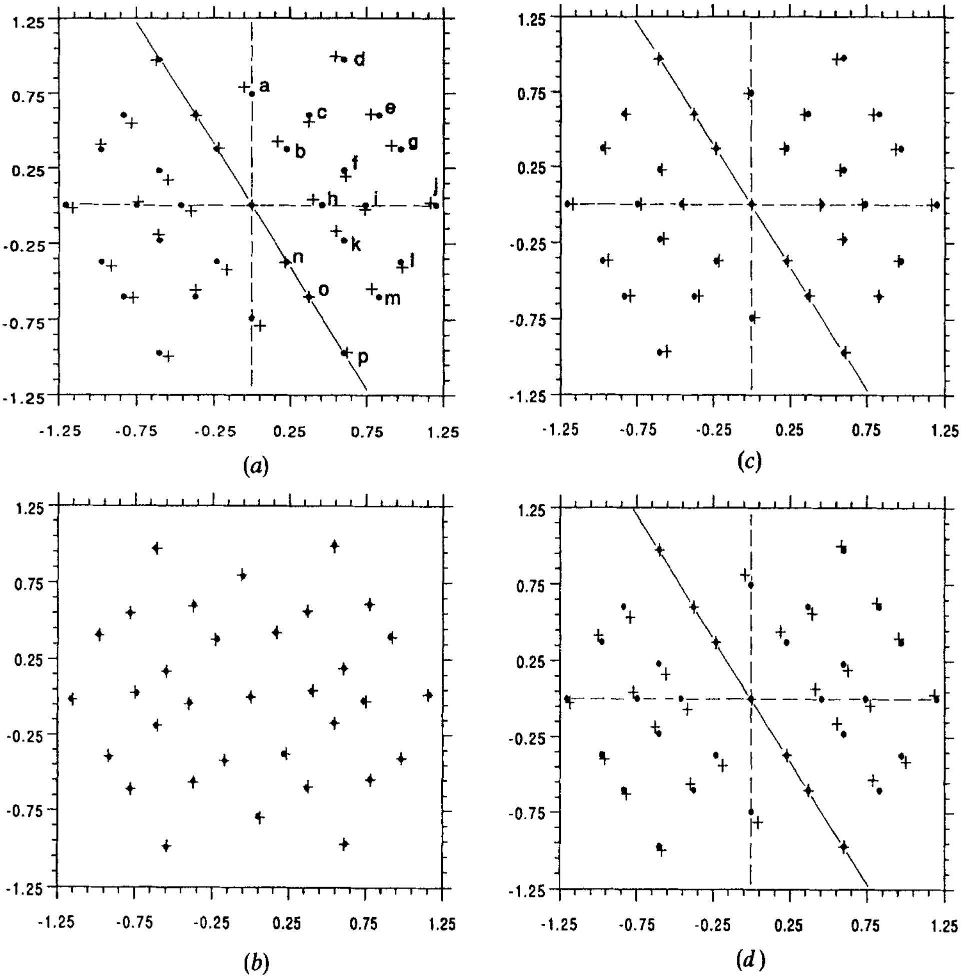
perpendicular to the common direction of a decagonal tenfold axis (A10) and an icosahedral fivefold axis (A5). In the epitaxial plane, twofold axes of the structure also have common directions. A detailed analysis of figs. 1 and 2 provides support for the following conclusions.

(1) The icosahedral phase is submitted to a certain strain field in the interface region. This appears as spot misalignments in the twofold zone axis diffraction pattern (fig. 1 (*c*′)) and fringe jags in the HREM dark-field micrograph (fig. 2).
(2) The observed strain field preserves the fivefold axis of the icosahedral phase which aligns parallel to the tenfold decagonal axis. This shows up in a comparison of the two parts of fig. 1 which differ only by rotation about the common axis.
(3) The corresponding strain field in the decagonal phase cannot be characterized.
(4) TEM observations on tilted interfaces have shown that they are dislocation free. This may thus suggest that the interface strain field relaxes via a phason- and/or phonon-like deformation.

§3. INTERPRETATION IN TERMS OF PHASON AND PHONON FIELD

The case of a single decagonal platelet in epitaxy on a semi-infinite icosahedral matrix is very difficult. Computer Fourier transforms of the corresponding HREM micrographs show that the epitaxy strain field progressively vanishes away from the interface. Instead, a simple uniform strain field may be expected if the icosahedral phase is reduced to a thin domain sandwiched in between decagonal platelets, as illustrated in fig. 2. In this high-resolution dark-field micrograph, white dots corresponding to the traces of fivefold plane families are visible. They are perfectly smooth when parallel to the interface but jag quasiperiodically otherwise.

Fig. 3



(*a*) (*c*) (*b*) (*d*)

(*a*) Comparison of reflection positions between those obtained from the computed Fourier transform of the central icosahedral sandwich shown in fig. 2 (+) and those of a perfect icosahedral quasicrystal (●): ---, twofold axes; ——, fivefold axis which can be considered as invariant. The letters correspond to those given in the table. (*b*) Comparison between the experimental reflections, shown previously in (*a*), and those calculated from the model. (*c*) Shifts of reflections produced by the phonon fields (see text). (*d*) Shifts of reflections produced by the phason fields (see text).

A computer Fourier transform of the sandwich image is shown in fig. 3 (*a*) and is compared with the pattern of a perfect icosahedral phase (for a rescaling with fig. 1 (*c*′), look at the spot labelled d in both diagrams). Invariance of the A5//A10 axis only is confirmed. The 'diffraction spots' of the strained icosahedral phase (fig. 3 (*a*)) have been given the indices of the closest reflection in the 'perfect-phase' pattern, according to the scheme proposed by Cahn, Shechtman and Gratias (1986). This is presented in the table, together with the corresponding $\mathbf{Q}^{/\!/}$ and $\mathbf{Q}^{\perp}$ modulis and the components $\Delta Q_x^{/\!/}$ and $\Delta Q_y^{/\!/}$ of the spot shift $\Delta\mathbf{Q}^{/\!/}$, with respect to the perfect-phase positions:

$$\Delta\mathbf{Q}^{/\!/}=\mathbf{Q}^{/\!/}_{\text{ico}}-\mathbf{Q}^{/\!/}_{\text{strained}}. \tag{1}$$

On the basis of theoretical models (Lubensky *et al.* 1986, Ishii 1989, Qiu and Jaric 1989), the $\Delta\mathbf{Q}^{/\!/}$ shifts may be analysed in term of a simple first-order linear phason and phonon strain field, such as

$$\Delta\mathbf{Q}^{/\!/}=\varepsilon^{/\!/\perp}\mathbf{Q}^{\perp}_{\text{ico}}+\varepsilon^{/\!/\,/\!/}\mathbf{Q}^{/\!/}_{\text{ico}}. \tag{2}$$

Phason–phonon coupling effects are neglected; $\varepsilon^{/\!/\perp}$ and $\varepsilon^{/\!/\,/\!/}$ are 2×2 matrices, since HREM can give only two-dimensional images of the strain field. The set of values $\Delta\mathbf{Q}^{/\!/}$, as expressed via eqn. (2), is adjusted to those deduced from experiment (table) using a refinement procedure first proposed by Simon, Lyon and de Fontaine (1985). The best fit has been obtained with

$$\begin{aligned}\varepsilon^{/\!/\perp}&=\begin{pmatrix}+0{\cdot}021\,94 & -0{\cdot}035\,08\\ -0{\cdot}023\,38 & +0{\cdot}050\,15\end{pmatrix}\\ &\approx k\begin{pmatrix}1 & \bar{\tau}\\ \bar{1} & \tau^2\end{pmatrix},\\ \varepsilon^{/\!/\,/\!/}&=\begin{pmatrix}+0{\cdot}027\,77 & -0{\cdot}026\,99\\ -0{\cdot}000\,34 & +0{\cdot}006\,42\end{pmatrix}\end{aligned} \tag{3}$$

Indexing of the icosahedral reflections shown in fig. 3 (*a*) and from which the reflection shift coordinates $\Delta Q_x^{/\!/}$ and $\Delta Q_y^{/\!/}$ observed with the deformed icosahedral phase have been determined.

Label	h/h'	k/k'	l/l'	Reflection symmetry	$Q^{/\!/}$ (Å^{-1})	$Q^{\perp}$ (Å^{-1})	$\Delta Q_x^{/\!/}$	$\Delta Q_y^{/\!/}$
a	0/0	2/0	0/0	30	0·724	1·172	0·051	−0·047
b	$\bar{1}$/1	1/0	0/0	12	0·426	1·114	0·061	−0·052
c	1/0	0/1	0/0	12	0·689	0·689	0·001	0·043
d	0/1	1/1	0/0	12	1·114	0·426	0·056	−0·020
e	$\bar{1}$/2	0/1	0/0	60	0·999	1·359	0·055	−0·006
f	0/1	$\bar{1}$/1	0/0	20	0·627	1·015	−0·009	0·037
g	1/1	1/0	0/0	20	1·015	0·627	0·059	−0·026
h	$\bar{2}$/2	0/0	0/0	30	0·448	1·896	0·059	−0·038
i	2/0	0/0	0/0	30	0·727	1·172	0·007	0·022
j	0/2	0/0	0/0	30	1·172	0·727	0·040	−0·017
k	0/1	1/$\bar{1}$	0/0	20	0·627	1·015	0·053	−0·059
l	1/1	$\bar{1}$/0	00	20	1·015	0·627	−0·009	0·036
m	$\bar{1}$/2	0/$\bar{1}$	0/0	60	0·999	1·359	0·049	−0·054
n	$\bar{1}$/1	$\bar{1}$/0	0/0	12	0·426	1·114	0·009	0·007
o	1/0	0/$\bar{1}$	0/0	12	0·689	0·689	0·001	−0·001
p	0/1	$\bar{1}$/$\bar{1}$	0/0	12	1·114	0·426	−0·018	−0·005

$$\approx k'\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \tag{4}$$

where k and k' are constants, *a priori*, depending on the icosahedral lattice parameter and on the hyperlattice deformation.

Using these two matrices to recalculate $\mathbf{Q}^{/\!/}_{\text{strained}}$ via eqns. (1) and (2) reproduces quite well the positions of the experimental spots (fig. 3 (*b*)). The effects of a phonon strain field alone ($\varepsilon^{/\!/ /\!/}$ matrix) and of a phason strain field alone ($\varepsilon^{/\!/\perp}$ matrix) are shown in figs. 3 (*c*) and (*d*) respectively. The phonon shifts (fig. 3 (*c*)) are weak, parallel to a twofold axis, antisymmetrically distributed with respect to the invariant fivefold direction $[\bar{1}\tau 0]$ and increase with increasing distance of the spot from the $[\bar{1}\tau 0]$ axis. Such phonon shifts, when expressed in direct space, correspond to an elastic strain field which induces a structural expansion. The phason shifts (fig. 3 (*d*)) are parallel and antiparallel to the $[\bar{1}\tau 0]$ direction, with a sign reversal every other spot row and they decrease with the distance of the spot from the invariant $[\bar{1}\tau 0]$ axis. Strictly speaking, the $[\bar{1}\tau 0]$ fivefold symmetry is not perfectly preserved by the phason matrix alone, as defined by eqn. (3). Had we had to achieve this invariance, this would imply that

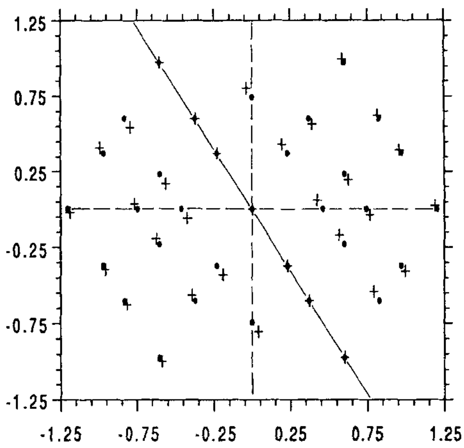
$$\varepsilon^{/\!/\perp} = k'\begin{pmatrix} 1 & \bar{\tau} \\ \bar{\tau} & \tau^2 \end{pmatrix}. \tag{5}$$

As illustrated in fig. 4, matrices (3) and (5) produce almost indistinguishable spot shifts. Considering that phonon–phason coupling has been neglected in the calculation of eqn. (3), and accounting also for some experimental inaccuracy (e.g. slight stigmatism of the HREM micrograph or limited resolution of the computer Fourier transform), this may suggest that matrix (3) has been mistakenly obtained instead of the better alternative matrix (5).

§ 4. WHAT ABOUT THE THREE-DIMENSIONAL PHASON FIELD?

As the icosahedral phase is a three-dimensional structure, any linear strain field and its corresponding matrix must be designed in three dimensions. Now the problem is to

Fig. 4



Effect of a phason matrix leaving one fivefold axis exactly invariant (see text); this figure should be compared with fig. 3 (*d*).

take, for instance, the matrix $\varepsilon^{/\!/\perp}$ as expressed in eqn. (5), to add one more horizontal row and one more vertical row of coefficients and to determine these extra coefficients with the requisite that the fivefold axial symmetry $[\bar{1}\tau 0]$ be preserved. Straightforward mathematical derivations demonstrate that this is just impossible; there is no solution whatsoever if the alleged three-dimensional $\varepsilon^{/\!/\perp}$ matrix is to be constructed to include the two-dimensional matrix (eqn. (3) or eqn. (5) are equally irrelevant in this respect). This suggests that the three-dimensional strain field is not uniform but may have linear two-dimensional components which are distributed quasiperiodically and preserve the axial A5–A10 symmetry. One possible model would be a phason strain field corresponding to *phason loops*. These phason loops (circular or decagonal) would be defined as the permissible trajectories for correlated phason atomic jumps. Because of symmetry requisites and to be consistent with the experimental observations, they should be sited in some planes parallel to the epitaxial interface. Such phason loops would indeed generate shifts of the diffraction spots in good consistency with those actually observed. More HREM observations are in progress to obtain support for the model.

§ 5. CONCLUSION

The strain field induced in a thin domain of an icosahedral phase by epitaxial coherent interfaces with a decagonal structure has been analysed. Uniform phason and phonon components of the strain field have been deduced from HREM micrographs, but the global three-dimensional fields cannot be linear in the physical space. A model for quasiperiodic phason and phonon fields has been suggested which must be supported by further experimental and theoretical developments.

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