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Structural variations in ϵ -type Al-Pd-(Mn, Fe) complex metallic alloy phases

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Abstract

Structural modifications in complex metallic ϵ -Al-Pd-(Mn, Fe) samples are studied by means of transmission electron microscopy. The modifications were observed in the vicinity of metadislocations and at phase boundaries. They are determined by the density and inclination of phason planes. In the vicinity of metadislocations and at an ϵ_6 - ϵ_{28} -phase boundary, new monoclinic ϵ -type structures appear locally, which were not detected as bulk phases in Al-Pd-(Mn, Fe) before. The present work points out the close entanglement between defects, i.e. metadislocations and phason planes, and structural modifications in ϵ -type complex metallic alloys. An extended classification of ϵ -type phases including monoclinic phases is presented on the basis of two different tiling descriptions.

Keywords: Transmission Electron Microscopy; Tiling; Metadislocation; Complex Metallic Alloys

§ 1. Introduction

Several structurally related orthorhombic phases have been identified as ternary extensions of the Al_3Pd phase in the Al-Pd-(Mn, Fe) alloy systems [1-9]. They are observed in a composition range extending from the binary Al_3Pd phase to about 5 % Mn and 10 % Fe [9] and are termed ε -phases. They are denoted ε_l ($l = 6, 16, 22, 28, 34^1$) according to the index of the strong $(0\ 0\ l)$ diffraction spot which corresponds to the interplanar spacing of about 0.2 nm occurring in all of those phases [7-9]. ε -type phases are also found in the alloy systems Al-Pd-(Rh, Re, Ru, Co, Ir) and Al-Rh-(Ru, Cu, Ni) [9, 10].

In the literature, ε_l -phases are sometimes referred to using alternative notations: The ε_6 - and ε_{28} -phases were denoted ξ' and Ψ , respectively [3-6]. Shramchenko and Denoyer [11] referred to the ε_6 -, ε_{16} -, and ε_{28} -phases as ξ' , ξ'_1 , and ξ'_3 . On the other hand, Engel [12] referred to these phases as ξ' , ξ'_1 , and ξ'_2 .

A particular feature of complex metallic ε -type phases is the occurrence of phase modulations and intermixing of structural elements. Modulated ε -type structures were observed in different alloy systems like Al_3Pd , $\text{Al}_{72}\text{Pd}_{25}\text{Cr}_3$, Al-Pd-Mn and Al-Pd-Fe [3, 10, 13].

In the present paper, structural modifications of ε -type phases in Al-Pd-(Mn, Fe) are studied by

means of transmission electron microscopy (TEM). We describe local structural modifications related to the density and inclination of phason planes occurring at a phase boundary between ϵ_6 - and ϵ_{28} -Al-Pd-Mn, where the phase boundary is built up by metadislocations. Furthermore structural alterations in the vicinity of metadislocations in ϵ -type Al-Pd-Mn and Al-Pd-Fe samples are studied. The presence of local unit cells corresponding to new monoclinic ϵ -type phases is reported. These phase modulations are discussed in terms of two tiling models. A generalized classification of ϵ -type structures is presented.

Structural description

The basic building blocks of all ϵ -phases are icosahedral-symmetric pseudo-Mackay clusters which are arranged in columns along the $[0\ 1\ 0]$ direction [4]. The projection of the column centres on the $(0\ 1\ 0)$ plane can be described in terms of so-called cluster tilings [1, 4, 14]. Two different tiles are used, a flattened hexagon H and a combination of a nine-edged banana-shaped polygon with a pentagon, termed phason line PL [3, 5]. Figure 1 a shows the H and PL tiles, which are present in two different orientations, denoted H1, H2, PL1, and PL2. Figure 1 b and c depict the tiling representations of the phases ϵ_6 and ϵ_{28} . These phases feature the orthorhombic space group Pnma and C2mm, respectively [4, 24]. The ϵ_6 structure can be described by alternating rows of H1 and H2 tiles [4]. The ϵ_{28} structure is characterised by additional PL1 tiles, which are aligned in rows along the $[1\ 0\ 0]$ direction (figure 1 c). An equivalent version of the ϵ_{28} structure can be constructed using PL2 tiles. All ϵ_i phases have identical $[1\ 0\ 0]$ and $[0\ 1\ 0]$ lattice constants, which, in the case of the Al-Pd-(Mn, Fe) alloy system, are $a = 2.35$ and $b = 1.66$ nm [4, 9]. The $[0\ 0\ 1]$ lattice constants of the ϵ_i phases differ. The lattice constants of the phases ϵ_6 and

¹ The ϵ_{34} phase was only observed in the alloy system Al-Pd-Mn [9].

ε_{28} are related by a factor $3 + \tau$, where $\tau = \frac{1}{2}(\sqrt{5} + 1)$ is the irrational number of the golden mean and $c(\varepsilon_6) = 1.23$ nm. Similar relations are found for other ε_l phases: The factor relating their [0 0 1] lattice constant to that of ε_6 are $1 + \tau$ (ε_{16}), $2 + \tau$ (ε_{22}), and $4 + \tau$ (ε_{34}).

In the present work all translation vectors are expressed in terms of the basis of ε_6 . Furthermore, we will use the term ε -type phases not only for the phase sequence ε_l ($l = 6, 16, 22, 28, 34$), but generalize it to all phases which can be described using the tiles H1, H2, PL1, and PL2 without creating gaps or overlaps. This includes also the so-called ξ phase, which is structurally closely related to ε_6 . It consists of a parallel arrangement of only one type of H tiles [4].

A mixture of structural elements belonging to different ε -type phases is observed in the vicinity of metadislocations. These metadislocations are a new type of structural defect, which was first observed in the ε_6 - and ε_{28} -phase [5, 15]. They are always associated to a certain number of planar defects, so-called phason planes. A phason plane in the ε_6 -phase can be structurally described by a row of PL-tiles along the [1 0 0] direction in an H-tile matrix. Since, on the other hand, a row of PL tiles is a structural element of the ε_{28} -phase (cf. figure 1 c), the presence of metadislocations leads to a mixture of structural features of the ε_6 - and the ε_{28} -phase [5, 16].

As an alternative to the cluster tiling involving H and PL tiles, other tilings can be used to describe the structure of ε -type phases. The *rhomb tiling* [3, 12] offers a simpler geometrical description than the cluster tiling. The relation between these alternative tilings is depicted in figure 2 a. The cluster-tiles H and PL have an even number of vertices. Therefore, the vertices can be divided into two disjoint sets (i.e. the cluster tiling is bipartite). By connecting the next-neighbours of one of those sets the alternative tiling is obtained: H1/H2 are substituted by the obtuse rhombs OR1/OR2, PL1 is substituted by a τ -inflated hexagon τ H, and PL2 is substituted

by a boat-shaped tile B (figure 2 a). This substitution is area-preserving, reversible and can be applied to any cluster tiling representing an ε -type phase. The tiles B and τH can be further decomposed into a combination of OR1, OR2, and an acute rhomb AR (figure 2 b). With this decomposition step, the cluster tiling can be substituted by a tiling using only obtuse and acute rhombs, OR1, OR2, and AR, and will then be referred to as a rhomb tiling [12]. The substitution of the tile τH by OR1, OR2, and AR, however, is not reversible as the back transformation is ambiguous. For the classification of ε -type phases in this paper, representations in terms of the cluster tiling and the rhomb tiling will be used.

In ε -type phases local rearrangements of cluster centres are possible. These can be represented in the cluster tiling by an exchange and $[0\ 0\ 1]$ displacement of PL1 and PL2 tiles (figure 2 c). This local movement of PL tiles, involving a correlated rearrangement of atomic clusters, is called a phason flip [3, 17]. Phason flips can also be described using the tiles OR1, OR2, B, and τH (figure 2 d) and the rhomb tiling (figure 2 e). In terms of the rhomb tiling, the distinction between PL1 and PL2 tiles is not possible (figure 2 e). Accordingly, the substitution of the second and third tiling of figure 2 c and d leads to equal rhomb tilings in figure 2 e.

§ 2. Experimental details

An ε_6 -Al-Pd-Mn single crystal was grown by means of the Bridgman technique. The final composition of the ingot was Al 73.6 at.%, Pd 22.1 at.%, Mn 4.3 at.%. It was characterised metallurgically and oriented by Laue diffraction. The undeformed sample was investigated by means of TEM and shows the presence of pure ε_6 -phase with a low density of defects like phason

planes. A sample of approximately $5 \times 2 \times 2 \text{ mm}^3$ in size was uniaxially deformed in compression to about 0.5 % strain. According to previous investigations on the plastic deformation properties of this material, the tests were performed in the ductile regime at a temperature of 700 °C. At temperatures below about 650°C the material is brittle [23]. The long specimen axis, corresponding to the compression direction, was oriented at an inclination of 45° with respect to the [0 1 0] direction in order to provide favourable conditions (i.e. a high Schmid factor) for metadislocation glide. The modes of metadislocation motion were discussed in detail by Feuerbacher and Heggen [22]. After mechanical testing the sample was quenched on a cold metal plate and prepared for TEM by standard techniques. The microstructural investigation was performed using a JEOL 4000 FX microscope and a Philips CM 200 FEG microscope equipped with a spherical-aberration corrector [18]. ϵ_6 - as well as ϵ_{28} -phase regions, formed during plastic deformation, were observed. The phase boundary region between both phases was analysed. Furthermore, structural modifications around metadislocations were analysed. A centric aperture around the direct beam and the central spots was used for imaging, which leads to enhanced contrast between phason-line elements and hexagon-type structural elements.

The second sample studied, an Al-Pd-Fe cast of the initial composition Al 64.4 at.%, Pd 34.8 at.%, Fe 1.5 at.%, was heat treated at 750 °C for 980 h. The material was characterised by scanning electron microscopy and TEM. The sample contains crystalline parts of ϵ -type phase with a composition Al 72.0 at.%, Pd 22.8 at.%, Fe 5.2 at.%. Lattice-fringe images under bright-field Laue conditions were taken in a JEOL 4000 FX microscope using a centric aperture around the direct beam and the central spots. The TEM samples were oriented along the [0 1 0] direction. In the present investigation two differently processed materials were compared: Plastically deformed single crystalline Al-Mn-Pd and cast polycrystalline Al-Mn-Fe. It is shown, however,

that the structural properties of metadislocations are not dependent on selective processing of the samples.

§ 3. Microstructural investigations

Figure 3 shows an electron micrograph of a phase boundary between the ϵ_6 - (left-hand side) and the ϵ_{28} -phase (right-hand side) in the Al-Pd-Mn sample. The ϵ_{28} -phase shows a darker contrast and the regular stacking of phason planes, visible as dark lines, can be seen in the rightmost part of the micrograph (cf. figure 1 c). The course of selected groups of phason-plane segments is indicated by curved lines. The phase boundary is formed by an almost straight-line arrangement of metadislocations along the $[0\ 0\ 1]$ direction. Exemplarily, the core of one metadislocation with 16 phason planes is indicated by an arrow. Another metadislocation, distant from the phase boundary by about 200 nm is indicated by an arrowhead. In the ϵ_{28} -phase, at a distance from the phase boundary the phason planes are oriented closely along the $[1\ 0\ 0]$ direction, while closer to the boundary they are mostly curved and inclined with respect to the $[1\ 0\ 0]$ direction.

Electron-diffraction patterns were taken in the vicinity of the phase boundary from three different regions, indicated by circles in figure 3. The sample regions a and c are located in the ϵ_6 - and ϵ_{28} -phase, respectively, and b corresponds to a region in the direct vicinity of the phase boundary on the ϵ_{28} -side, about 50 nm distant from the metadislocations. The corresponding diffraction patterns are shown in figure 4. The insets show enlargements corresponding to the area marked by a rectangle in figure 4 a. For a closer inspection of the diffraction patterns, figures 4 b and c show additionally further enlarged segments. The diffraction patterns 4 a and c confirm the presence of the ϵ_6 - and ϵ_{28} -phase. The corresponding $(0\ 0\ 6)$ and $(0\ 0\ 28)$ reflections are marked. Diffraction pattern b resembles that of the ϵ_{28} -phase but it is not identical. For a closer inspection

of the reflection positions, four diffraction spots are marked by circles in figure 4 c. These positions are transferred to the inset in figure 4 b (circles). The low-intensity diffraction spots in the inset of figure 4 b show slight deviations with respect to position and intensity from those of the ϵ_{28} -phase.

Figures 5 a and b show high-resolution micrographs of the Al-Pd-Mn sample in two regions close to the ϵ_6 - ϵ_{28} -phase-boundary corresponding to area b in figure 3. The micrographs were taken at an overfocus of about 40 nm in order to emphasise the large spatial frequencies, which gives rise to bright-contrast dots at the centres of the pseudo-Mackay clusters. A tiling representation of these areas using H1, H2, PL1, and PL2 tiles can then easily be made by connecting the bright dots. The tilings which consist of semi-transparent white H1 and H2 and red PL1 and PL2 tiles are superimposed to the micrographs. In the tiling representation of figure 5 a, the unit-cell projection of the ϵ_{28} -phase is represented by a rectangle. Over large areas of the micrograph, however, the ϵ_{28} -structure is disordered. Phason planes are not strictly oriented along the [1 0 0] direction but show a wavy course due to mixing of PL1 and PL2 tiles within a single phason plane (e.g. regions 1 and 2 in figure 5 a). This observation can be explained by the occurrence of phason flips within a phason plane (cf. figure 2 c). In some areas the phason planes are inclined, i.e. a (1 0 1) translation can be found between neighbouring equal PL tiles (arrows). Along the [0 0 1] direction a varying number of H1 and H2 tiles is observed between two PL tiles, ranging from 0 to 3 in figure 5 a (examples are indicated by circles).

In figure 5 b an average separation of phason planes larger than in the ideal ϵ_{28} -phase is observed. Locally, a rectangular cell is spanned by the vectors (1 0 0) and (0 0 4+ τ) representing the ϵ_{34} -phase (rectangle in figure 5 b). At the top right part of figure 5 b two neighbouring PL tiles of a phason plane are related by a (1 0 2) translation (arrow). In some areas even stronger inclinations

between PL tiles are observed.

A lattice fringe image of the same sample showing structural modifications around metadislocations is presented in figure 6. Four metadislocations (labelled 1 to 4) are connected to ϵ_6 -phase regions (labelled 5 to 8) [5]. Phason lines are visible as dark features. The course of selected groups of phason-plane segments is indicated by curved lines. They show a variable inclination with respect to the $[1\ 0\ 0]$ direction. For example, in an area close to the ϵ_6 -phase region (labelled 9) phason planes join, which have a negative and positive slope with respect to the $[1\ 0\ 0]$ direction. Furthermore, a variable density of phason planes is observed in terms of their mutual distance along the $[0\ 0\ 1]$ direction. The variation of the phason plane density is introduced due to the presence of metadislocations. These metadislocations terminate phason planes and therefore lead to an unidirectional compaction of the latter. As an example, phason planes terminating at a the metadislocation labelled 3 are indicated by curved lines in figure 6. The phason plane density on the left hand side of the metadislocation is much higher than at the right hand side. In addition to the phason planes, a stacking fault (10) is observed on the right hand side of figure 6. This type of defect was discussed by Klein *et al.* [15], but is not a matter of discussion in the present investigation.

The local structure of some selected areas in this sample region is analysed in figure 7 a to c, which depict enlargements of the boxed regions of figure 6. Within areas of 10 to 20 nm in diameter, homogeneous local structures are observed, which can be matched by tilings. In figure 7 a, a space-filling tiling is made using PL and H tiles. The corresponding unit cell is spanned by the vectors $(1\ 0\ 0)$ and $(0\ 0\ 3+\tau)$. This local structure can therefore be identified as ϵ_{28} phase. The local structure in figures 7 b and c is characterised by inclined phason planes and different numbers of H1 and H2 tiles between the phason planes. The unit cell is spanned by the vectors $(1$

0 -1) and (0 0 4+ τ) (figure 7 b), and (1 0 1) and (0 0 6+ τ) (figure 7 c), respectively. The angle between those vectors is 108° and 72° rather than 90°. The lattice can therefore be considered a monoclinic rather than an orthorhombic lattice.

A similar structural study was made using an Al-Pd-Fe sample. Figure 8 shows a lattice fringe image in the vicinity of metadislocations (labelled 1 and 2), which are connected to ξ -phase regions (labelled 3 and 4) [19]. The course of selected groups of phason-plane segments is indicated by curved lines. Again, they show a variable inclination with respect to the [1 0 0] direction, and a variable density of phason planes is observed. Figures 9 a to c depict enlargements of the boxed regions in figure 8, which are matched by cluster tilings. In figure 9 a the corresponding unit cell is spanned by the vectors (1 0 0) and (0 0 1+ τ). This local structure can be identified as ε_{16} phase. In figures 7 b and c the unit cell is spanned by the vectors (1 0 -1), (0 0 4+ τ) and (1 0 -1), (0 0 2+ τ), respectively.

§ 4. Discussion

Microstructural investigations

In this paper, a TEM study on structural modifications in complex metallic ε -type phases is presented. These structural modifications are connected to phason defects and metadislocations and occur on different length scales. For instance, figures 5 a and b show structural modifications, i.e. phason flips, on the scale of the lattice parameter. Single PL elements exhibit a modulated behaviour within the phason planes which are, on average, oriented along the [1 0 0] direction. Beyond that, figure 3, 6, and 8 demonstrate that structural modulations exist on a larger

scale ranging from some tens to hundreds of nanometres. They depend on the curvature and density of phason planes in these areas.

On the unit-cell scale, local structural disordering was observed at an ϵ_6 - ϵ_{28} -phase boundary by means of high-resolution TEM. Various distances between phason planes along the $[0\ 0\ 1]$ direction and the local occurrence of other unit cells (e.g. ϵ_{34}) were found. The average structure in the vicinity of the phase boundary has a larger separation between the phason planes than the perfect ϵ_{28} -phase. Single PL elements are moved out of regularly stacked $(0\ 0\ 1)$ planes by phason flips which results in a wavy course of the phason planes (figure 5). In addition, the electron diffraction investigation reveals structural modulations in the direct vicinity of the phase-boundary region. The shifts of spots can be related to the presence of phason disorder [20, 21].

On a larger scale structural modifications are connected to the course of phason planes which are observed as dark lines in figure 3. Metadislocations terminating the phason planes are not ideally stacked along $[0\ 0\ 1]$ direction, but may be distant from the boundary along the $[1\ 0\ 0]$ direction (see arrowhead in figure 3). Accordingly, the density of phason planes varies locally and, on average, increases gradually from the ϵ_6 - to the ϵ_{28} -phase region. As ϵ -type phases within a sequence ϵ_l ($l = 6, 16, 22, 28, 34$) are distinguished by their $[0\ 0\ 1]$ lattice constants, i.e. the distance between phason planes along the $[0\ 0\ 1]$ direction, the variation of the phason plane distance due to the presence of metadislocations is associated with local structural variations. No sharp phase boundary but rather a transient region is observed between related ϵ -type phases. The intermediate region is characterized by a variation of the phason plane density leading to a continuous phase change and the presence of phason disorder.

Structural modulations connected to the course of phason planes were furthermore investigated in the vicinity of metadislocations in an Al-Pd-Mn and an Al-Pd-Fe sample (figures 6 to 9). Due to

the presence of metadislocations, phason planes are geometrically forced to circumvent defected areas (for example the ones labelled 8 in figure 6). This gives rise to various phason-plane inclinations with respect to the $[1\ 0\ 0]$ direction. Furthermore, the introduction of additional phason planes by metadislocations (for example the ones labelled 3 in figure 6) causes a local variation of the phason plane density and to a local structural variation within the sequence of ε_l -phases ($l = 6, 16, 22, 28, 34$). The structural variations around the metadislocations are found in both samples investigated here, the plastically deformed single crystalline Al-Mn-Pd and cast polycrystalline Al-Mn-Fe sample. These observations are not dependent on selective processing of the samples.

The observation of phason plane inclinations with respect to the $[1\ 0\ 0]$ direction leads a structural description in terms of a tiling model which is elaborated in the following subsection. These local phason plane inclinations can be described in terms of monoclinic ε -type structures. The discussion in terms of monoclinic structures is based on the structural investigation within the $(0\ 1\ 0)$ -plane. Potential structural changes along the $[0\ 1\ 0]$ -direction are not considered. Monoclinic ε -type bulk phases have not been observed in the Al-Pd-(Mn, Fe) alloy system before.

An important characteristic regarding structural modifications connected to metadislocations in ε -type phases is the mutual sense of the terms “defect” and “structural element”. Phason planes associated with metadislocations are defects, but, on the other hand, they are elements of the ideal structure in all ε -type phases but ε_6 . In this sense, the presence of defects is always necessarily connected to structural variations of the surrounding material and to the local appearance of new monoclinic structures around the defects.

Classification of ε -type phases

In figure 10, a systematic classification scheme for ε -type orthorhombic and monoclinic phases is presented. PL1 and PL2 tiles are depicted white, H1 and H2 tiles dark grey and light grey, respectively. The presented ε -type structures are characterized by different periodic arrangements of straight phason planes. They differ with respect to their inclination along the $[1\ 0\ 0]$ direction and their spacing along the $[0\ 0\ 1]$ direction.

The central column of the figure represents the tilings of the orthorhombic ε -phases. From top to bottom we find ε_{16} , ε_{22} , ε_{28} , ε_{34} , and ε_{40} . Their lattice vectors, expressed in terms of the basis of ε_6 (cf. §1; the basis vectors are shown in figure 2b), are given by $(1\ 0\ 0)$ and $(0\ 0\ z+\tau)$, $z = 1, 2, 3, 4, 5, \dots$. The first, second, fourth, and fifth column of figure 10 show ε -type tilings of monoclinic structures spanned by $(1\ 0\ -2)$, $(1\ 0\ -1)$, $(1\ 0\ 1)$, and $(1\ 0\ 2)$ translation vectors, respectively. Note that the structures in corresponding columns on the left and right hand side are related by a mirror operation. Tilings shown in the same row possess the same translation vector along the $[0\ 0\ 1]$ direction; tilings in the same column possess the same inclination of phason planes.

The tilings shown in figure 10 can be classified by two indices (m, n) according to the translation vectors $(0\ 0\ m+1+\tau)$ and $(1\ 0\ n)$, with $m = 0, 1, 2, 3, \dots$ and $|n| \leq m$. The index n is confined corresponding to the latter relation in order to avoid overlap of the tiles. For reasons of presentation, the phases $(3, -3)$, $(4, -3)$, $(4, -4)$, etc. were not shown in figure 10. Orthorhombic and monoclinic phases are classified by the indices $n = 0$ and $n \neq 0$, respectively. The ε_6 -phase and the ξ -phase, consisting only of H tiles, can be expressed in terms of the present classification as the limit of an infinite distance between the phason planes, i.e. by the indices $(n, 0)$ and $(n, \pm n)$ for $n \rightarrow \infty$, respectively.

In terms of this classification, the orthorhombic structures shown in figure 7 a and 9 a correspond to the orthorhombic phases referred to as (2,0) and (0,0). The monoclinic structures depicted in figure 7 and 9 can be assigned to the structures (3,-1) (figure 7 b and fig. 9 b), (4,1) (figure 7 c), and (1,-1) (figure 9 c). It should be noted that the enlarged areas in figure 7 and 9 were selected to show locally undistorted ε -type structures which can be classified according to the scheme of figure 10. In these areas, the local structures remain constantly ordered over distances of several lattice parameters. The intermediate ranges between such areas show mixing of structural elements of related ε -phases. The same holds for areas showing heavily curved phason planes around metadislocations or rapidly changing phason-plane density at phase boundaries. These local changes take place by a high density of phason flips.

Hiraga [13] studied decagonal and quasicrystalline phases by high-resolution electron microscopy in Al-Pd-(Cr, Co, Fe). He observed modulated ε -type structures, which can be classified according to our scheme. The areas shown in figure 11 of Hiraga's work can be identified as (3,1), (2,-1), (2,0), and (0,0) [13].

A comparable classification can be created in terms of the rhomb tiling. The unit cell is spanned by the basis vectors **a** and **c**, while **b** is the (fixed) basis vector perpendicular to the tiling plane. The vectors **a** and **c** are given by integer linear combinations of the three vectors $\mathbf{e}_i$, $i = 1, 2, 3$, that span the rhomb tiles OR, AR (cf. figure 2). In contrast, the edges of the cluster tiling are described by a regular five-star basis. In this sense the rhomb tiling is a geometrically simpler description than the cluster tiling. The vector **c** connects two PL tiles in the [0 0 1] direction, while the vector **a** connects two next-neighbouring PL tiles along or inclined with respect to the [1 0 0] direction. In the $\{\mathbf{e}_i\}$ basis they are

$$\mathbf{c} = \begin{pmatrix} 1 \\ 2+m \\ 1 \end{pmatrix} \text{ and } \mathbf{a} = \begin{pmatrix} 1 \\ n \\ -1 \end{pmatrix} . \quad (1)$$

The classification in terms of the rhomb tiling is shown in figure 11. OR1 and OR2 tiles are depicted white and AR tiles grey. The parameter m specifies the distance of the phason planes, and the parameter n the inclination of the phason planes with respect to the $[0\ 0\ 1]$ direction. The lattice constants a , c , and their angle ϕ can be calculated as a function of m , n :

$$c/\lambda = \tau + 1 + m, \quad (2)$$

$$a/\lambda = \sqrt{n^2 + 2 + \tau}, \quad (3)$$

$$\tan \phi = \frac{\sqrt{2 + \tau}}{n}, \quad (4)$$

for $n \neq 0$ and $\lambda = c(\varepsilon_6) = 1.23$ nm. For $n = 0$ $\phi = 90^\circ$ holds.

The number of the H1, H2, and PL tiles per unit cell is $\#(\text{H1}) = m + n$, $\#(\text{H2}) = m - n$, $\#(\text{PL}) = 2$.

The parameters m , n can be determined by counting the relative densities of the tile types:

$$m = \frac{\#(\text{H1}) + \#(\text{H2})}{\#(\text{PL})}, \quad n = \frac{\#(\text{H1}) - \#(\text{H2})}{\#(\text{PL})}. \quad (5)$$

A direct consequence of these relations is the restriction $|n| \leq m$.

It should be noted that the phases of the present classification scheme represent “simple” phases which can be built with the tiles H1, H2, PL1, and PL2 in the sense that they are described by two translation vectors connecting PL tiles. This results in structures which are characterised by a uniform distribution of straight phason lines. However, more complex periodic phases using H and PL tiles can be constructed, e.g. by the creation of supercells of the presented simple phases.

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Figure captions

- Figure 1: Hexagon H1/H2 and phason-line tiles PL1/PL2 (a) are the basic building blocks of ε -type phases; examples are the ε_6 -phase (b) and the ε_{28} -phase (c).
- Figure 2: (a) The cluster tiles (light grey) can be substituted by the tiles OR1/OR2, τ H, and B. (b) The tiles τ H and B (grey) can be further decomposed into obtuse rhombs OR1/OR2 and acute rhombs AR. Local rearrangements of tiles (phason flips) can be formed in the cluster tiling (c), the tiling using the tiles OR1/OR2, τ H, and B (d), and the rhomb tiling (e).
- Figure 3: Transmission electron micrograph of a phase boundary in Al-Pd-Mn formed by metadislocations between the ε_6 -phase on the left and the ε_{28} -phase on the right hand side. Phason planes associated to the metadislocations can be observed as dark lines. One metadislocation is marked by an arrow. Diffraction patterns were taken at the sample areas a, b, and c.
- Figure 4: Diffraction patterns of the sample areas a, b, and c of figure 3. The insets show enlarged images of the boxed section.
- Figure 5: High resolution micrographs of an Al-Pd-Mn sample in the ε_{28} -phase region close to the ε_6 - ε_{28} -phase-boundary. The corresponding cluster tilings are superimposed to the micrographs.
- Figure 6: Lattice fringe image of an Al-Pd-Mn sample containing four metadislocations (1 to 4) connected to ξ -phase regions (5 to 8). The course of phason planes is exemplarily indicated by curved line elements (9, see text). In addition a stacking fault is observed (10). Enlarged images of the boxed regions are presented in figure 7.

Figure 7: Enlarged sections of the areas marked a, b, and c in figure 6. The local structure is matched by three different cluster tilings.

Figure 8: Lattice-fringe image of an Al-Pd-Fe sample containing two metadislocations (1 and 2) connected to ξ -phase regions (3 and 4). The course of phason planes is exemplarily indicated by curved line elements. Enlarged images of the boxed regions are presented in figure 9.

Figure 9: Enlarged sections of the areas marked a, b, and c in figure 8. The local structure is matched by three different cluster tilings.

Figure 10: Classification of ε -type phases using the cluster tiling. The phases are characterized by two indices (m, n) with $m = 1, 2, 3, \dots$ and $|n| \leq m$. See text.

Figure 11: Classification of ε -type phases using the rhomb tiling. The tilings of figure 10 and 11 are related by a substitution.

Hexagon H1/H2 and phason-line tiles PL1/PL2 (a) are the basic building blocks of ϵ -type phases; examples are the ϵ_6 -phase (b) and the ϵ_{28} -phase (c).

419x131mm (72 x 72 DPI)

(a) The cluster tiles (light grey) can be substituted by the tiles OR1/OR2, τH , and B. (b) The tiles τH and B (grey) can be further decomposed into obtuse rhombs OR1/OR2 and acute rhombs AR. Local rearrangements of tiles (phason flips) can be formed in the cluster tiling (c), the tiling using the tiles OR1/OR2, τH , and B (d), and the rhomb tiling (e).

411x242mm (72 x 72 DPI)

Figure 3: Transmission electron micrograph of a phase boundary in Al-Pd-Mn formed by metadislocations between the ϵ_6 -phase on the left and the ϵ_{28} -phase on the right hand side. Phason planes associated to the metadislocations can be observed as dark lines. One metadislocation is marked by an arrow. Diffraction patterns were taken at the sample areas a, b, and c.

529x385mm (72 x 72 DPI)

Figure 5: High resolution micrographs of an Al-Pd-Mn sample in the ϵ_{28} -phase region close to the ϵ_6 - ϵ_{28} -phase-boundary. The corresponding cluster tilings are superimposed to the micrographs.

Lattice fringe image of an Al-Pd-Mn sample containing four metadislocations (1 to 4) connected to ξ -phase regions (5 to 8). The course of phason planes is exemplarily indicated by curved line elements (9, see text). In addition a stacking fault is observed (10). Enlarged images of the boxed regions are presented in figure 7.

667x472mm (72 x 72 DPI)

Figure 7: Enlarged sections of the areas marked a, b, and c in figure 6. The local structure is matched by three different cluster tilings.

Lattice-fringe image of an Al-Pd-Fe sample containing two metadislocations (1 and 2) connected to ξ -phase regions (3 and 4). The course of phason planes is exemplarily indicated by curved line elements. Enlarged images of the boxed regions are presented in figure 9.

447x417mm (72 x 72 DPI)

Figure 9: Enlarged sections of the areas marked a, b, and c in figure 8. The local structure is matched by three different cluster tilings.

Classification of ε -type phases using the cluster tiling. The phases are characterized by two indices with $m = 1, 2, 3, \dots$ and $|n| \leq m$. See text.

582x1062mm (72 x 72 DPI)

Classification of ϵ -type phases using the rhomb tiling. The tilings of figure 10 and 11 are related by a substitution.
623x1061mm (72 x 72 DPI)