# Tiling models for metadislocations in AlPdMn approximants

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**Abstract**

The AlPdMn quasicrystal approximants $\xi$, $\xi'$, and $\xi'_n$ of the 1.6 nm decagonal phase and $R$, $T$, and $T_n$ of the 1.2 nm decagonal phase can be viewed as arrangements of cluster columns on two-dimensional tilings. We substitute the tiles by Penrose rhombs and show, that alternative tilings can be constructed by a simple cut and projection formalism in three dimensional hyperspace. It follows that in the approximants there is a phasonic degree of freedom, whose excitation results in the reshuffling of the clusters. We apply the tiling model for metadislocations, which are special textures of partial dislocations.

## 1 Introduction

A quasiperiodic structure can be described as a cut through a hyperlattice decorated with atomic surfaces. As a consequence the atoms are arranged in a finite number of different local environments frequently leading to a substructure of highly symmetric clusters. The cluster positions can again be modelled by a simpler decoration consisting in the simplest case of exactly one atomic surface (for the cluster centre) per hyperlattice unit cell. The displacement of the cut space (phasonic displacement) is a discrete degree of freedom, called phasonic degree of freedom. It can be excited locally, leading to a rearrangement of the clusters by correlated atomic jumps. This view is supported by recent diffraction data of coherent phason modes in i(cosahedral)-AlPdMn (Coddens et al. 1999, Francoual et al. 2003) and by in situ observations of phason jumps via high-resolution transmission electron microscopy (HRTEM) in d(ecagonal)-AlCuCo (Edagawa et al. 2002).

The cut formalism cannot be applied directly if there is a gradient in the phasonic displacement. This is examplified by the extreme case of a cut space running inbetween

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all atomic surfaces and not touching any of them. Hence we resort to another method: We substitute the atomic surfaces by atomic hypervolumes (Engel and Trebin 2005) of the same dimension as the hyperspace. For the construction two different spaces are needed: Those atomic hypervolumes that are cut by the (possibly deformed) cut space $E_{\mathrm{Cut}}$ are selected. The centre of each selected atomic hypervolume is projected onto the projection space $E_{\mathrm{Proj}}$. By shearing the cut space, i.e. by introducing a linear phasonic displacement, periodic approximants are created. Phasonic degrees of freedom also can exist in these and play a fundamental role for phase transitions (Edagawa et al. 2004).

Here we discuss linear defects, metadislocations, in the phasonic degree of freedom for approximants of the AlPdMn system. This system is especially adequate for the examination of phasonic degrees of freedom since a stable i-phase, a stable 1.2 nm d-phase, a metastable 1.6 nm d-phase (which is assumed to be a solid solution of Mn in d-AlPd (Steurer 2004)), and a large variety of approximants have been observed in the phase diagramm (Klein et al. 2000). All of them, as well as several binary AlPd and AlMn quasicrystals and approximants are related structurally.

## 2 Tiling models

A hyperspace model for i-AlPdMn has been proposed by Katz and Gratias (1993). It uses a six dimensional face-centred hyperlattice $F^{6D}$ with lattice constant $2l^{6D} = 1.29$ nm and serves as a starting point since to our knowledge all newer, more complicated hyperspace models are refinements. It has been shown, that the approximants $\xi$ and $\xi'$ (Beraha et al. 1997) of the 1.6 nm d-phase and the approximants $R$ and $T$ (Beraha et al. 1998) of the 1.2 nm d-phase are described on an atomistic level by a shear in this model. However the authors had to introduce an additional mirror symmetry to assure full tenfold symmetry. The main building units are Mackay-type clusters, whose centres are projected from the hyperspace by using one atomic surface per hyperlattice unit cell. It is a subset of a triacontahedron, deflated by $\tau = \frac{1}{2}(\sqrt{5}+1)$ with respect to the canonical triacontahedron, which is the projection of the hypercube with edge length $l^{6D}$ on the orthogonal complement of $E_{\mathrm{Proj}}$. The distance of the cluster centres is the shortest projection of neighboring $F^{6D}$-sites $\boldsymbol{e}_i \pm \boldsymbol{e}_j$ multiplied by the deflation factor: $t^{6D} = \frac{1}{5}\sqrt{10}\sqrt{\tau+2}l^{6D} \simeq 0.78$ nm.

The relation of the approximants to the i-phase is given by two consecutive shears of $E_{\mathrm{Cut}}$ in the hyperspace: The first shear changes the cluster arrangement in direction of a fivefold axis $\boldsymbol{e}_1$. Together with the introduction of a mirror plane this results in a decagonal quasicrystal. The clusters are then aligned in columns parallel to the tenfold axis, so that the structures can be described by two-dimensional tilings, which are the projections in the column direction. The second shear rearranges the columns perpendicular to $\boldsymbol{e}_1$. We will now consider the tilings for the 1.6 nm and the 1.2 nm phases separately.

Neighboring clusters in the 1.6 nm d-phase and its approximants lie on planes perpendicular to $\boldsymbol{e}_1$. Thus the tile length is $t^{6D}$ as defined above. The $\xi$- and the $\xi'$-phase are built from flattened hexagons (H) arranged in parallel and in alternated orientation respectively. By introducing additional rows of pentagons (P) and nonagons (N) between

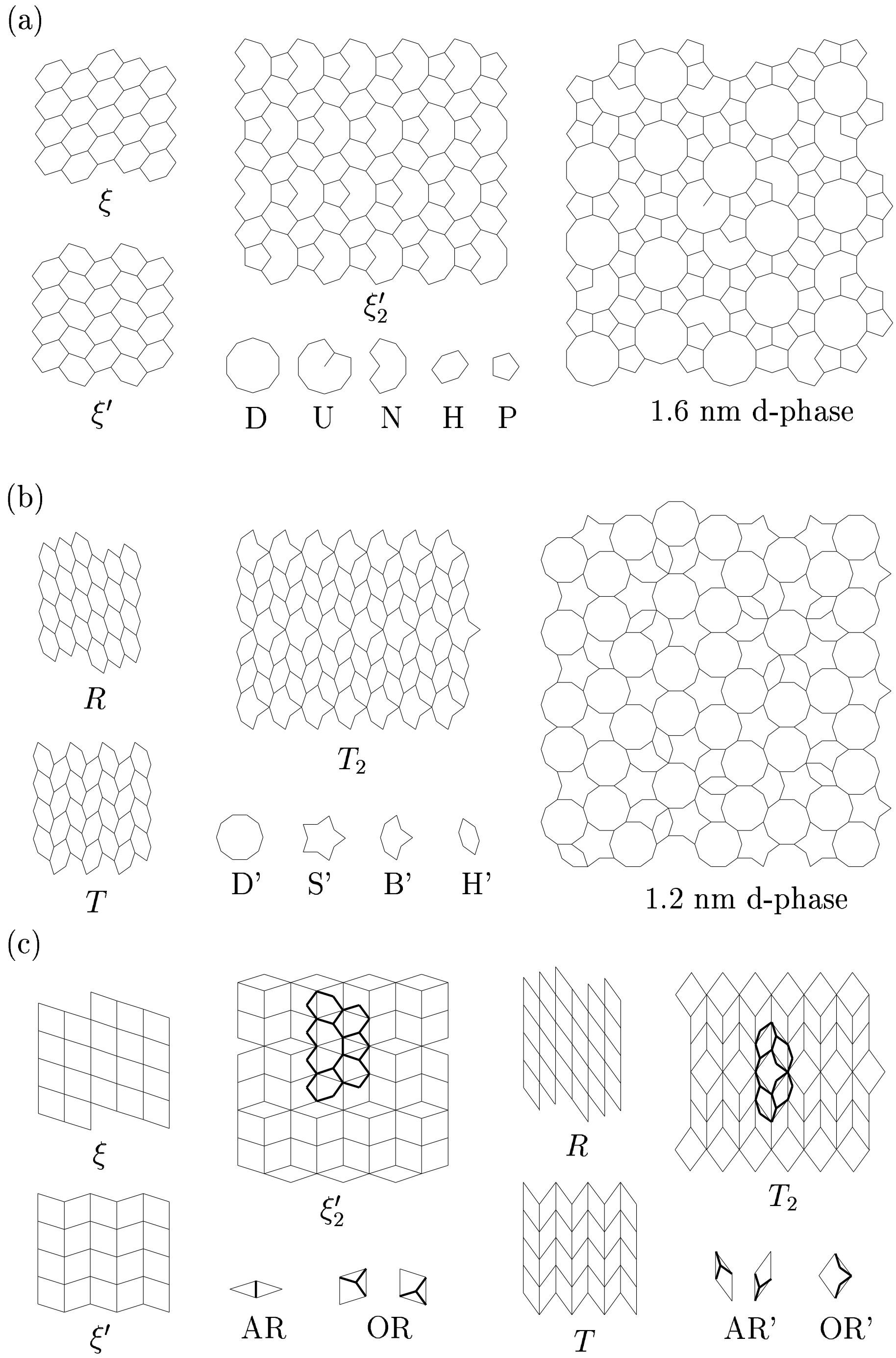


Figure 1: Calculated tilings for various approximants of the AlPdMn i-phase. (a) 1.6 nm phases: The tiling of the d-phase is the Tübingen Triangle Tiling (TTT). (b) 1.2 nm phases: The D' centers lie on a $\tau^2$ inflated TTT. (c) The tiles can be substituted with Penrose rhomb tiles. The substitution is different for the 1.6 nm phases and the 1.2 nm phases.

each $n-1$ rows of alternated Hs in the $\xi'$-phase we obtain the $\xi'_n$-phases. Such a PN-row is called a phason plane, which is justified since it is elongated in the $\boldsymbol{e}_1$ direction. As we will see, phason planes play an important role for the cluster reshuffling resulting from an excitation of the phasonic degree of freedom. Further tiles, the decagon (D) and an U-shaped tile (U) are observed in the 1.6 nm d-phase (Fig. 1 (a)).

Neighboring clusters in the 1.2 nm d-phase and its approximants lie on two planes staggered perpendicular to $\boldsymbol{e}_1$ with distance $\frac{1}{5}\sqrt{10}l^{6D} \simeq 0.41$ nm. The resulting tile length is $t'^{6D} = \frac{1}{5}\sqrt{10}\tau l^{6D} \simeq 0.66$ nm. The $R$- and the $T$-phase are built from elongated hexagons (H') arranged in parallel and in alternated orientation respectively. The $T_n$-phases are created by introducing into the $T$-phase additional rows of boat-shaped tiles (B') between each $n$ rows of alternated H's. A B'-row is again called a phason-plane. For the 1.2 nm d-phase additionally a decagon (D') and a star-shaped tile (S') are needed (Fig. 1 (b)).

By substituting the H, P, N, H', and B' tiles with acute rhombs (AR), (AR') and obtuse rhombs (OR), (OR') as shown in Fig. 1 (c) we obtain new tilings for the approximants, which can be interpreted as approximants of the Penrose-tiling. An H is substituted by an OR, while a phason plane corresponds to a combination of an AR-row and an OR-row. So the $\xi'_n$-phase has $n$ OR-rows inbetween neighboring AR-rows. Similarly the $T_n$-phase has $n$ AR-rows inbetween neighboring phason planes, represented by OR-rows. The rhombs occuring in the new tilings for the $\Xi$-approximants ($\xi$, $\xi'$, $\xi'_n$), as well as for the $T$-approximants ($R$, $T$, $T_n$) both only need three of the five basis vectors of the Penrose-tiling to be constructed. Therefore the tilings can be modelled in a simple three-dimensional hyperspace with the $\mathbb{Z}^3$-lattice and lattice constant $l^{3D} = \tau\sqrt{\tau+2}l^{6D} \simeq 1.99$ nm. The projection matrices are ($s_i = \sin(2\pi\frac{i}{5})$, $c_i = \cos(2\pi\frac{i}{5})$):

$$\pi^{||}_{\Xi} = \frac{1}{5}\sqrt{10}\begin{pmatrix} s_0 & s_1 & s_4 \\ c_0 & c_1 & c_4 \end{pmatrix}, \qquad \pi^{||}_{T} = \frac{1}{5}\sqrt{10}\begin{pmatrix} s_0 & s_2 & s_3 \\ c_0 & c_2 & c_3 \end{pmatrix}, \tag{1}$$

leading to an edge length of the tiles: $t^{3D} = \frac{1}{5}\sqrt{10}l^{3D} \simeq 1.26$ nm. There is one atomic hypervolume per unit cell, which is just the unit cell, and one phasonic degree of freedom. This three-dimensional hyperspace is the simplest model for a phasonic degree freedom besides the Fibonacci-chain.

# 3 Metadislocations

In the formalism of atomic hypervolumes a dislocation can be introduced into a tiling by a generalised Voltera process (Engel and Trebin 2005). It is uniquely characterised by a translation vector of the hyperlattice, the Burgers vector $\boldsymbol{b}$ (here: $\boldsymbol{b}^{3D} = (b_1, b_2, b_3)$, $b_i \in \mathbb{Z}$), that splits up into a phononic component $\boldsymbol{b}^{||} = \pi^{||}\boldsymbol{b}$ (deforming the tiles) and a phasonic component $\boldsymbol{b}^{\perp}$ (rearranging the tiles). The latter can only be calculated from the full six-dimensional Katz-Gratias model. If it is not zero, such a dislocation is a partial dislocation. By (i) extending the linear theory of elasticity to the hyperspace, (ii) approximating the phasonic degree as continuous, and (iii) assuming isotropy in the strain fields, the line

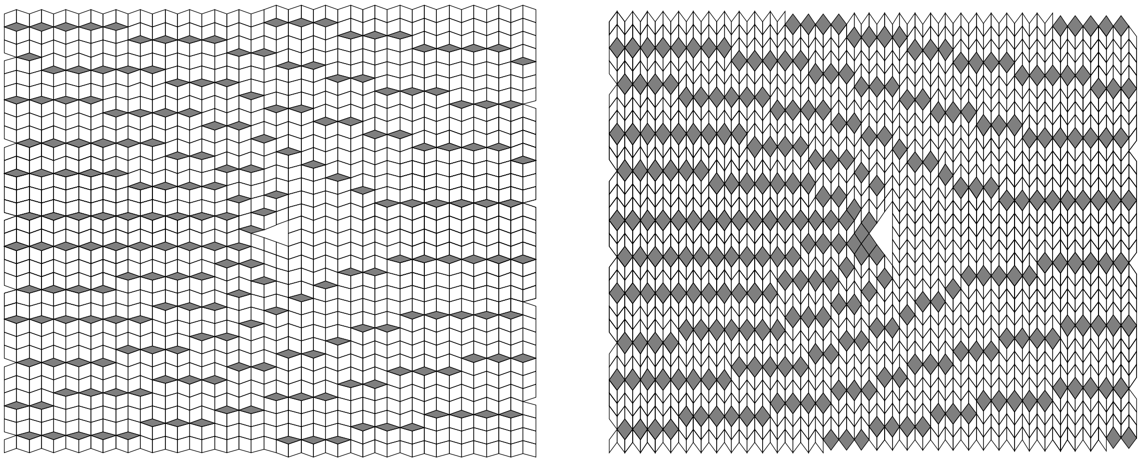

Figure 2: Tilings of the $\xi_3'$- (left) and the $T_3$-phase (right) with $m = 4$ metadislocations. $2F_m$ new phason planes are inserted from the left, ending at the triangular shaped dislocation core.

energy $E$ of a dislocation is expressed as:

$$E = c_{\mathrm{phon}} \|\boldsymbol{b}^{||}\|^2 + c_{\mathrm{phas}} \|\boldsymbol{b}^{\perp}\|^2 + c_{\mathrm{coupl}} \|\boldsymbol{b}^{||}\| \|\boldsymbol{b}^{\perp}\|. \tag{2}$$

Besides a phononic contribution with material constant $c_{\mathrm{phon}}$ and a phasonic contribution with $c_{\mathrm{phas}}$, a coupling term is present with $c_{\mathrm{coupl}}$. According to experiment we assume $c_{\mathrm{phon}} \gg c_{\mathrm{phas}} \approx c_{\mathrm{coupl}}$. Since stable dislocations are those with the lowest energy, we have to minimise $\|\boldsymbol{b}^{||}\|$. We will discuss this in parallel for dislocations in the $\Xi$- and the $T$-approximants. The minimization yields $b_2 = b_3$ in both cases. Furthermore we have $b_1 = -\tau^{-1} b_2$ for $\boldsymbol{b}_{\Xi}^{3D}$ and $b_1 = \tau b_2$ for $\boldsymbol{b}_T^{3D}$. Here we approximate $\tau^{-1}$ by the fractions $F_{m-1}/F_m$ and $\tau$ by the fractions $F_{m+1}/F_m$ respectively. $(F_m)_{m \in \mathbb{N}}$ are the Fibonacci numbers with start values $F_1 = F_2 = 1$. Finally the Burgers vectors of stable dislocations are: $\boldsymbol{b}_{\Xi}^{3D} = (F_{m-1}, -F_m, -F_m)$ and $\boldsymbol{b}_T^{3D} = (F_{m+1}, F_m, F_m)$. Interestingly they correspond to the same six-dimensional Burgers vectors:

$$\boldsymbol{b}_{\Xi}^{6D} = \boldsymbol{b}_T^{6D} = (0, 0, -F_{m-2}, F_{m-1}, F_{m-2}, F_{m-1}). \tag{3}$$

Hence it suffices to consider both cases together for the rest of our calculations. The phononic component $\boldsymbol{b}^{||} = \boldsymbol{b}_{\Xi}^{||} = \boldsymbol{b}_T^{||}$ is perpendicular to the phason-planes (in the vertical direction in Fig. 1). We get $\|\boldsymbol{b}^{||}\| = \tau^{-m} t^{3D}$ and $\|\boldsymbol{b}^{\perp}\| = \tau^{m-3} t^{3D}$. Substituting this into (2), we have $E = \left[c_{\mathrm{phon}} \tau^{-2m+3} + c_{\mathrm{phas}} \tau^{2m-3} + c_{\mathrm{coupl}}\right] \tau^{-3} (t^{3D})^2$. There is a minimum for $c_{\mathrm{phon}}/c_{\mathrm{phas}} = \tau^{4m-6}$. This determines the Burgers vector with lowest energy for given values for the material constants $c_{\mathrm{phon}}$ and $c_{\mathrm{phas}}$. However it has to be noted that these are not necessarily identical for the $\Xi$- and the $T$-approximants.

Tilings of the $\xi_3'$- and the $T_3$-phase with $m = 4$ dislocations have been calculated (Fig. 2). They show large rearrangements of the tiles due to the phasonic component $\boldsymbol{b}^{\perp}$

and negligible deformations of the tiles due to the smaller phononic component $\boldsymbol{b}^{\|}$. The dislocations are also dislocations in the metastructure of the phason planes. Therefore Klein et al. (1999), who discovered these dislocations in HRTEM images of the $\xi_2'$-phase, named them metadislocations. The fact, that the experimentally most often observed metadislocations are those with $m = 4$ suggests $c_{\text{phon}}/c_{\text{phas}} = \tau^{10} \simeq 123$. We do not know of Burgers vector determinations or observations of metadislocations in the $T$-approximants, but dislocations with the Burgers vectors (3) are also the ones most often observed in the i-phase (Rosenfeld et al. 1995).

# 4 Discussion and conclusion

In the $\xi_n'$- and the $T_n$-phases the phasonic degree of freedom is related to the movement of the phason planes. Since there are no phason planes in the $\xi$-, $\xi'$-, $R$-, and $T$-phase, the phasonic degree of freedom cannot be excited locally. However metadislocations can exist in the $\xi'$- and the $T$-phase, but not in the $\xi$- and the $R$-phase. It can be shown, that there is no consistent way to introduce dislocations with phasonic components in the latter phases.

A motion of the metadislocation (like the motion of any dislocation in a quasicrystal or large unit cell approximant) is necessarily accompanied by diffusion in the form of tile rearrangements. The motion is possible by climb in direction of the phason planes or by glide perpendicular to them. During the climb motion new phason planes are created (or dissolved) behind the dislocation core. A large number of metadislocations moving through the $\xi'$- or $T$-phase could even lead to a phase transformation to the $\xi_n'$- or $T_n$-phases making the phasonic degree of freedom continously excitable. This is affirmed by HRTEM images of phase boundaries between the $\xi'$- and the $\xi_2'$-phase formed by metadislcations (Heggen and Feuerbacher 2005).

On the other side, glide motion does not change the number of phason planes. At least in the $\xi'$- and the $T$-phase glide motion seems unprobable, since the phason planes running out of the dislocation core would have to be dragged along, while climb motion only needs a reconstruction of the tiling near the dislocation core. (Similar arguments leading to the same conclusion, as well as newer experimental work are presented in Feuerbacher and Heggen (2005).) We have to note, that there are no direct observations of metadislocation motion in approximants yet, although in the i-phase dislocations with identical Burgers vectors have been shown by in-situ observations to move by climb (Mompiou et al. 2004).

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