Model Quasilattice for Al-Mn Decagonal Quasicrystal

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A model quasilattice for the Al-Mn decagonal quasicrystal is proposed. It is a periodic stacking of two-dimensional pentagonal quasilattices with the period $c = 1.24$ nm. The space group is $P10_5/mmc$ and the one period is written as CC where C is a composite layer with the point group D_{5h} and $\bar{C}$ is related to C by the screw axis 10_5 . The composite layer C is composed of five layers as $B_2B_1AB_1B_2$ and the central layer A is on the mirror plane. The layers B_1 and B_2 form the puckered layer $B = B_1B_2$ and C is written as B^*AB with B^* ($= B_2B_1$) being the mirror image of B . The layer A is obtained by decorating a pentagonal variation of the Penrose tiling with pentagons, stars, boats and thin rhombi and the remaining two layers, B_1 and B_2 , are two-dimensional quasilattices decorating the pentagonal Penrose tiling.

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I. Introduction

The structure determinations of decagonal quasicrystals (DQCs) are urgent subjects⁽¹⁾⁻⁽⁹⁾. A DQC is a periodic stacking of a few types of quasiperiodic layers along the c -axis, i.e., the axis of the ten-fold rotation. Some of the layers are flat but others puckered. There exist several polytypes with respect to the stacking periods. The interlayer spacing is common among different DQCs and equal to $c_0 = 0.2$ nm. The period c is an even multiple of c_0 ⁽¹⁰⁾. A representative DQC with $c/c_0 = 2, 4, 6$ or 8 is Al-Cu-Co, Al-Ni-Co, Al-Mn or Al-Fe, respectively.

A model of the atomic structure of a quasicrystal (QC) is given by the quasilattice (QL) which is a quasiperiodic set of points in the physical space⁽⁵⁾⁽¹¹⁾. In particular, each layer of the DQC is modeled by a two-dimensional (2D) QL with the decagonal symmetry D_{10} (10 mm) or the pentagonal one D_5 (5 m). A decagonal quasilattice (DQL) is obtained in the section method[†] as a 2D section of a hypercrystal, which is a 4D periodic structure with the decagonal symmetry⁽⁵⁾⁽¹¹⁾⁽¹²⁾. The 2D space E_2 embedding the DQL is called the physical space and the orthogonal complement $E_2^\perp$ the internal space. The hypercrystal is obtained from a 4D decagonal lattice L by locating the atomic surfaces (ASs) on its lattice points. An AS is a polygon parallel to $E_2^\perp$, so that its section through E_2 is a point. If there exist two or more lattice points per one unit cell of L , different ASs are assigned to different sublattices into which L is divided. An AS has the same point symmetry as that of the relevant sublattice⁽¹³⁾ and ASs assigned to equivalent sublattices differ only in their orientations in $E_2^\perp$. The translational symmetry of L is represented by a Bravais lattice L_0 and L is divided into

sublattices which are translationally congruent to L_0 . A QL (exactly, the relevant local-ismorphism class) is specified by L_0 , L and the ASs.

A QL is divided into several sublattices corresponding to those of L . The sites of a sublattice are different sections of the AS assigned to it and the sections are distributed uniformly and densely in the AS. Consequently, the density of the sites in E_2 is proportional to the area of the AS⁽¹⁴⁾.

L_0 is easily determined by the symmetry of the diffraction pattern and the position of a high-intensity reflection in it, while L and ASs are determined by analyzing the intensities of different reflections⁽⁵⁾. However, the ASs determined by the diffraction experiment are diffuse on account of the phason disorder and violate the exclusion conditions forbidding site pairs whose distances are smaller than a value allowed as an interatomic distance. In order to obtain an ideal model QL, we have to correct the diffuseness by using other information obtained by the HREM, the EXAFS, the density measurement, etc.

A QC has usually one or more approximant crystals⁽¹⁵⁾⁽¹⁶⁾, which have similar local atomic structures to the QC. If the atomic structure of an approximant is determined by a diffraction experiment, it limits strongly the sizes and forms of the ASs of the associated QC. The model QL for a QC is, however, not uniquely determined from the structure of its approximant crystal because the approximant includes only limited local structures of the QC or, in other words, it surveys only limited points of the ASs. The boundaries of the ASs can usually be varied to some extent without changing the structure of the approximant lattice.

The ASs of Al-Cu-Co and Al-Mn have been roughly determined by Steurer by means of X-ray diffraction experiments on single crystals⁽⁴⁾⁽⁶⁾. Burkov⁽⁷⁾ proposed for Al-Cu-Co a good model QL which is consistent with Steurer's ASs and the HREM by Hiraga *et al.*⁽¹⁷⁾. For Al-Ni-Co, Yamamoto *et al.*⁽³⁾ proposed a model QL on the basis of an X-ray diffraction experiment on a single

[†] The section method is equivalent to the projection method⁽¹¹⁾. A window is assigned in the latter method to each sublattice. Each window is exactly equal to the inversion of the corresponding atomic surface in the section method.

crystal. Their sample had, however, a stacking disorder and the period of the average structure was $2c_0$, i.e., half the ideal value. Li and Kuo⁽⁹⁾ proposed a structural model for Al-Mn on the basis of the structure of the approximant crystal $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$. Their model was presented as a decoration of the Penrose tiling with rhombic tiles and L as well as the ASs have not been given explicitly.

Recently, Hiraga *et al.*⁽¹⁸⁾ determined the structure of Al_3Mn which is an approximant to Al-Mn DQC. The aim of the present paper is to propose a structural model for Al-Mn based on this work as well as the diffraction experiment⁽⁶⁾. The properties of the 4D decagonal lattices^{(12)(13)(19)–(22)} are reviewed in Section II. Several DQLs are introduced in Section III. In Section IV, a model QL for Al-Mn is proposed and its features are investigated. Section V is devoted to discussions and conclusions.

II. The 4D Decagonal Lattices^{(12)(13)(19)–(22)}

Let us take a 4D decagonal lattice L which is a Bravais lattice. The point group of L is obtained by lifting the 2D point group D_{10} (10 mm) up to the 4D and is isomorphic to the latter. Therefore, an 2D operation in D_{10} and its 4D version are represented by the same symbol, e.g., C_{10} for the ten-fold rotation. The two-fold rotation C_2 is the inversion operation not only in the 2D but also in the 4D: $C_2 = -1$. Note that C_{10} and C_2 have the same effect when operated on an object with the five-fold rotational symmetry.

It is convenient for L to take a symmetrical but over-complete set of basis vectors ε_i , $i=0-4$, with $\sum_i \varepsilon_i=0$; four of ε_i , e.g., ε_i , $i=1-4$, form a complete set. We shall adopt the convention $\varepsilon_i = \varepsilon_{i+5}$, so that the suffix i belongs to the finite field $Z_5 \equiv \{0, 1, 2, 3, 4\} (=Z/5Z)$. Let e_i and e'_i be the components of ε_i in E_2 and E'_2 , respectively. Then, they are written as $e_i = a(\cos(2\pi i/5), \sin(2\pi i/5))$ and $e'_i = a'(\cos(4\pi i/5), \sin(4\pi i/5))$, where a (or a') is the lattice constant in the physical (or internal) space. a' is nothing to do with the properties of the QL derived from L , so that two lattices which differ only in the value of a' are considered to be identical. The five-fold rotation C_5 ($=C_{10}^2$) acts onto E'_2 as a rotation through $4\pi/5$.

A lattice vector of L is uniquely indexed with five integers $l = \sum_i n_i \varepsilon_i \equiv [n_0 n_1 n_2 n_3 n_4]$ provided that the condition $0 \leq \sum_i n_i \leq 4$ is imposed on n_i , which we assume hereafter:

$$L = \left\{ \sum_{i=0}^4 n_i \varepsilon_i \mid n_i \in Z, 0 \leq \sum_{i=0}^4 n_i \leq 4 \right\}. \quad (1)$$

The value $\sum_i n_i$ is called the level of the relevant lattice vector. The level is considered to belong to Z_5 . The level of the sum $l+l'$ of two lattice vectors l and l' is equal to the sum of the levels of l and l' . From (1), L is divided naturally into five sublattices L_p , $p \in Z_5$, on different levels; $L = L_0 \cup L_1 \cup L_2 \cup L_3 \cup L_4$. We will sometimes equate L_3 and L_4 with L_{-2} and L_{-1} , respectively, because $3 \equiv -2$ and $4 \equiv -1 \pmod{5}$. L_p are translationally equivalent; $L_p = x_p + L_0$, where $x_1 = \varepsilon_0$, $x_2 = \varepsilon_2 + \varepsilon_3$, x_3

$(=x_{-2}) = -x_2$ and $x_4 (=x_{-1}) = -x_1$ are representative lattice vectors of L_p . More generally, $L_{p+q} = l + L_q$ if $l \in L_p$.

The sublattice L_0 is written as

$$L_0 = \left\{ \sum_{i=0}^4 n_i \varepsilon_i \mid n_i \in Z, \sum_{i=0}^4 n_i = 0 \right\}, \quad (2)$$

which is a superlattice of L . It is virtually similar to L ; this expression can be changed into a similar form to (1) by using the new bases $\delta_i = \varepsilon_{i+2} - \varepsilon_{i+3}$. The physical-space lattice constant of L_0 is given by $a_0 = 2a \sin(\pi/5)$, while its axes in E_2 are rotated through $\pi/10$ from those of L .

The space group of L_0 is a semi-direct-product of the translational group L_0 and the 4D decagonal point group D_{10} . The sublattices L_p are special points of L_0 with the point group D_5 (5 m); $C_5 L_p = L_p$, $p=1-4$. The two sublattices L_1 and L_4 (or L_2 and L_3) are equivalent with respect to L_0 and are interchanged each other by C_2 and C_{10} . Let us define $\bar{L}_p \equiv -L_p$ ($=C_2 L_p$), $p=0-4$. Then, we obtain $\bar{L}_p = L_{-p}$ and, in particular, $\bar{L}_0 = L_0$.

L and L_0 are invariant against the volume-conserving affine transformation, $T = \tau I \oplus \tau' I$ with $\tau = (1 + \sqrt{5})/2$ being the golden ratio and $\tau' = -1/\tau$; T scales E_2 and E'_2 by τ and τ' , respectively. Note that $TL_p = L_{3p}$. T gives rise to a self-similarity of a QL derived from L or L_0 .

The 4D reciprocal lattice L_0^* to L_0 is given by λL with $\lambda = 2/(5a^2)$, so that it is similar to L . The real space component G of each lattice vector of L_0^* is indexed uniquely with the basis vectors $e_i^* = a^*(\cos(2\pi i/5), \sin(2\pi i/5))$, $i=0-4$, as $G = \sum_i m_i e_i^* = (m_0 m_1 m_2 m_3 m_4)$, $0 \leq \sum_i m_i \leq 4$, where $a^* = 2/(5a)$ ($=\lambda a$).

III. The Decagonal Penrose QL and a Pentagonal One

The 2D QL associated with the Penrose tiling with pentagons is obtained from L_0 by assigning a decagonal AS⁽²⁰⁾ whose vertices are at $\pm(e'_{i+2} - e'_{i+3})$, $i=0-4$, i.e., the projections of $\pm\delta_i$ onto E'_2 . The edge length of the pentagons is equal to a_0 . We shall identify the QL with the Penrose tiling associated with it. It is a decagonal QL although it has no local centres of the ten-fold rotational symmetry. The QL includes not only the pentagons but also stars, boats and thin rhombi.

The once inflated version of the Penrose tiling is obtained by using a shrunken AS which is τ^{-1} -times the original one⁽²⁰⁾. The edge length of the inflated tiles is given by $d = 2a \sin(2\pi/5)$ ($=\tau a_0$). For a convenience of a later argument, we shall refer to this tiling and the QL associated with it as the decagonal Penrose QL. The centres of the pentagons in the QL are local centres of the five-fold rotational symmetry. They are the projections of the lattice points of L_2 and L_3 ; the two sublattices refer to the two orientations of the pentagons⁽¹³⁾⁽²⁰⁾.

Let us modify the decagonal AS into a pentagonal one which is a union of five smaller decagons as shown in Fig. 1; the areas of the two ASs are the same. The 2D QL derived with the new AS is shown in Fig. 2. It is, surprisingly, composed of the same tiles as those of the original QL, i.e., the Penrose tiling. However, the point

Fig. 1 The AS of a pentagonal modification of the Penrose tiling with pentagons (solid lines). The AS is the union of the five decagons. The larger decagon in broken lines is the AS of the original Penrose tiling, which is decagonal. The horizontal (or vertical) direction is parallel (or perpendicular) to e'_0 in E'_2 .

Fig. 2 Pentagonal modifications of the Penrose tilings with pentagons (solid lines) and rhombi (broken lines). The two tilings are locally related to each other.

symmetry of the QL is pentagonal. In fact, stars assume only one of the two possible orientations and boats five of ten. These orientations of the tiles shall be called positive ones. On the other hand, pentagons can assume both the two orientations but the number density is different between the two. The majority orientation shall be called the positive one and the minority the negative one. The circumferential pentagons of stars assume the positive orientation. The same is true for the circumferential pentagons of boats except those touching the bottoms of the boats. The present QL is a pentagonal variation of the Penrose tiling and we shall call it the pentagonal Penrose QL. It will be denoted by Q_0 and its AS by S_0 .

As shown in Fig. 1, S_0 is divided into ten sub-ASs, five of which are thin hexagons and the other five the concave octagons. The five hexagons are associated with the vertices which are shared by two positive pentagons, e.g. the convex vertices of stars, and refer to the five orientations of the relevant type of vertices. Other vertices are grouped into the second type, which is associated with the octagons. The ratio of the number densities of the two types of vertices is estimated from the areas of the sub-ASs, resulting $\tau:2$.

The number density of the vertices of Q_0 is given by $\rho_0 = 1/(d^2 \sin(2\pi/5))$ and that of the positive pentagons by $\rho_0/(\sqrt{5}\tau)$. The relative ratios of the number densities of the positive pentagons, negative ones, rhombi, boats and stars are $1:\tau^{-1}:\tau^{-2}:\tau^{-5}:\tau^{-4}$.

IV. A Model QL for the Al-Mn DQC

Al-Mn is a DQC with the stacking period $c=6c_0$, so that one period is composed of six layers⁽²⁾. The space group is $P10_5/mmc$ ⁽²⁾. Since the c axis is the axis of the screw axis 10_5 , the space group has no centres with the ten-fold rotational symmetry. One period of Al-Mn includes two horizontal mirror planes, which are related to each other by the screw axis. The point group of the mirror planes is $D_{5h}(10m2)=D_5 \times C_s$ with $C_s=\{E, \sigma_h\}$ being the mirror group.

We shall review next the structure of Al_3Mn , an approximant to Al-Mn⁽¹⁸⁾. Al_3Mn has the orthorhombic unit cell with dimensions $a=1.483$ nm, $b=1.243$ nm and $c=1.251$ nm and the space group is $Pnma$. The b -axis is the pseudo-decagonal axis which corresponds to the c -axis of Al-Mn. Al_3Mn has a layered structure with layers perpendicular to the b -axis. One period is equal to $6c_0$ and is composed of six layers as represented by $B^*AB\bar{B}^*\bar{A}\bar{B}$; layers X and $\bar{X}$ are related by the n glide, while B and B^* by the mirror through the layer A . Therefore, the structure of Al_3Mn is specified by those of A and B . A (or $\bar{A}$) is flat because it is on a mirror plane. The puckered layer B (or B^*) is divided into two sublayers as B_1B_2 (or $B_2^*B_1^*$); the sublayers are almost flat. The sublayer B_1 has only the Al sites but A and B_2 have both the Al and Mn sites.

The layer A has ten Al sites per a $2D$ unit cell. Eight of them form a periodic tiling of regular pentagons and thin rhombi; the unit cell contains four pentagons and two rhombi. The tiling is considered to be a periodic approximant to the decagonal or pentagonal Penrose tiling. Other sites in the layer A or those in B_1 and B_2 decorate the pentagons symmetrically but the rhombi asymmetrically. The real positions of atoms in Al_3Mn shift slightly from the ideal sites described here. We assume that the layers B_1 and B_2 are flat in the ideal structure. Then, $B^*=B_2B_1$. A model QL for Al-Mn will be constructed on the ideal structure. The successive interlayer spacings in the stacking $\cdots AB_1B_2B_2\cdots$ are .155 nm, .075 nm and .161 nm. This completes a review of the structure of Al_3Mn determined by Hiraga *et al.*⁽¹⁸⁾.

A model QL for Al-Mn is obtained by replacing the layers A , B_1 and B_2 in Al_3Mn by their quasiperiodic versions, which are pentagonal⁽⁹⁾. We shall denote the quasiperiodic layers by the same symbols as those of their periodic versions. We assume that the periodic tiling in the layer A of Al_3Mn is a periodic approximant to Q_0 , the pentagonal Penrose QL shown in Fig. 2. Then, the QL provide us with the basic structure of Al-Mn. The $2D$ QLs representing other sites in the layers A , B_1 and B_2 are determined by the condition that they decorate the tiles in the basic structure in the same way as

in Al_3Mn . Our model QL is a periodic stacking of 2D QLs and the stacking rule is the same as that of Al_3Mn . The 2D QLs A , B_1 and B_2 are given as $A = Q_0 + Q_4 + Q'_2$, $B_1 = Q_1 + Q_3$ and $B_2 = Q_2$, where Q_p , $p=1-4$, are 2D QLs obtained from L_p by assigning the ASs, S_p , $p=1-4$, shown in Fig. 3, while Q'_2 is a sublattice of Q_2 associated with the central sub-AS of S_2 . The AS S_3 is star-shaped but is not similar to the star tile in Q_0 . The lattice constants of the model QL are $a = .251$ nm, $c = 1.24$ nm and $d = .478$ nm. A and $\bar{A}$ are on mirror planes, which are related by the screw axis 10_5 . One period of the model QL is written as $CC\bar{C}$, where $C \equiv B^*AB (=B_2B_1AB_1B_2)$ is a composite layer with the point symmetry D_{5h} . This expression explicitly shows the space group, $P10_5/\text{mmc}$. The layers A and B are shown in Fig. 4.

We shall consider how the tiles of the basic QL, Q_0 , are decorated by other 2D QLs[†]. First, Q'_2 or Q_3 decorates the centres of the positive or negative pentagons, respectively. The ASs of other QLs are divided into sub-ASs as shown in Fig. 3 so that different types of sub-ASs yield different decorations of Q_0 . The five circumferential decagons of S_1 or stars of S_2 and S_4 refer to quintets decorating positive or negative pentagons, respectively; the quintets from S_2 and those from S_4 decorate the pentagons differently. The hexagonal sub-ASs of S_2 and S_4 as well as the central sub-AS of S_1 refer to decorations of stars, boats and rhombi. As shown in Fig. 3, the central sub-AS of S_1 is divided further into eleven smaller sub-ASs, i.e., a small decagon, five arrows and five kites. The decagon refers to the sublattice decorating the centres of stars in Q_0 , while the arrows (or kites) to the decoration of the boats (or rhombi).

The relative ratios of the number densities of the 2D

Fig. 3 The ASs assigned to sublattices L_p , $p=1-4$. The ASs (a), (b), (c) and (d) are S_p , $p=1-4$, in this order. The edges are parallel to e'_i , $i=0-4$, and their lengths are the same, which is equal to $\tau^{-2}a'$. Each AS is divided into sub-ASs associated with the sublattices which decorate the QL in Fig. 2 in different ways.

[†] We can see the relationships between different QLs introduced in this paper if we copy them on transparent sheets and superpose the copies.

QLs, Q_p , $p=0-4$, and Q'_2 are given by $(\tau+2):(\tau+4):(4\tau-1):\tau^{-1}:(4\tau-2):1$. The number density of a sublattice of each 2D QL is calculated from the area of the relevant sub-AS. Note in this respect that the relative ratios of the areas of the decagonal sub-AS, the star and the thin rhombus are $\tau:1:1/\sqrt{5}$.

The sublattice $Q_{12} \equiv Q_1 + Q_2$ of the layer B yields a tiling with stars, thin hexagons and concave octagons as shown in Fig. 5. The bond length is equal to a . This tiling is similar to a decagonal sublattice of the Penrose tiling with rhombic tiles⁽¹³⁾. In fact, Q_3 (or Q_0) divides the stars (or octagons and hexagons) in Q_{12} into rhombi resulting a quasiperiodic tiling with the same two types of rhombi as those of the rhombic Penrose tiling. This tiling has ten-pronged vertices where ten thin rhombi meet. It is a generalized rhombic Penrose tiling but different from those investigated by Pavlovitch and Kléman⁽²³⁾. On the other hand, the layer A yields a quasiperiodic tiling with decagons, stars and thin hexagons: The decagons are unions of two thin hexagons and one concave octagons. The decagons are centred by the sites from Q'_2 . The three quasiperiodic tilings introduced here are not decagonal but pentagonal.

Another generalized rhombic Penrose tiling is obtained from $Q'_{123} \equiv Q'_1 + Q'_2 + Q_3$, where Q'_1 is a sublattice of Q_1 derived from the central sub-AS, i.e., the star, of S_1 . The rhombi of this tiling are τ^3 times as large as those of the previous one but the two tilings are not similar. This tiling is locally related to Q_0 as shown in Fig. 2. The sites of sublattices Q'_2 and Q_3 are located on the centres of the positive and negative pentagons of the pentagonal Penrose tiling Q_0 , respectively, and $Q_{2,3} \equiv Q'_2 + Q_3$ yields a tiling with stars, concave octagons and thin hexagons, which are locally related to stars, boats and thin rhombi of Q_0 , respectively. The sites of Q'_1 induce divisions of the three types of the tiles of $Q_{2,3}$ into rhombi. A similar relation is known between the original Penrose tiling with pentagons and the rhombic Penrose tiling (or its decagonal sublattice)⁽¹³⁾⁽²⁴⁾. Each of the 2D QLs Q_p , $p=0-4$, and Q'_2 decorates the two types of rhombi of Q'_{123} in its own rule (see, for example, Fig. 5). The rules of the decorations by the layers A and B are the same as those proposed by Li and Kuo⁽⁹⁾. As a matter of fact, the hexagons in the tiling $Q_{2,3}$ are the building blocks of the two approximants Al_3Mn and $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ ⁽²⁵⁾.

The layers $\bar{A}$ and $\bar{B}$ are composed of 2D QLs, $\bar{Q}_p$, $p=0-4$, and $\bar{Q}'_2$, which are obtained from $\bar{L}_p (=L_{-p})$ and $\bar{L}_2$ by assigning the ASs $\bar{S}_p \equiv -S_{-p}$ and $\bar{S}'_2 \equiv -S'_2$ to them. The majority pentagons, stars and boats of the pentagonal Penrose tiling $\bar{Q}_0$ assume negative orientations. Q_0 and $\bar{Q}_0$ do not overlap perfectly because $S_0 \neq \bar{S}_0$. $\tilde{S}_0 \equiv S_0 \cup \bar{S}_0$ is a regular decagon and $\bar{Q}_0 \equiv Q_0 \cup \bar{Q}_0$ yields a decagonal tiling as shown in Fig. 6, which includes new tiles of thick rhombi in addition to the old ones. Stars and boats of Q_0 (or $\bar{Q}_0$) overlap with rhombi of $\bar{Q}_0$ (or Q_0) but with no stars nor boats. Some of the majority pentagons in Q_0 and $\bar{Q}_0$ overlap partially resulting thick rhombi in $\bar{Q}_0$. On the other hand, the minority pentagons in Q_0 (or $\bar{Q}_0$) overlap perfectly with parts of the majority

Fig. 4 The profiles of the layer $A (= Q_0 + Q_4 + Q_2')$ (a) and the layer $B (= Q_1 + Q_2' + Q_3)$ (b). (a) The spots, double circles and simple ones show the sublattices Q_0 , Q_2' and Q_4 , respectively. The sublattice Q_0 form a pentagonal Penrose tiling shown by the dashed lines whose length is equal to the lattice constant $d (=4.78 \text{ nm})$. The five spots decorating a pentagon are derived from the five star-shaped sub-ASs of S_4 . (b) The pentagonal Penrose tiling show the sublattice Q_0 of the neighbouring A layer. The double circles, simple ones and spots show the sublattices Q_1 , Q_2 and Q_3 , respectively. Of the circles, those centred on positive pentagons are derived from the central sub-AS of S_2 . The five double (or simple) circles decorating a pentagon are derived from the five decagonal (or starshaped) sub-ASs of S_1 (or S_2).

Fig. 5 A quasiperiodic tiling with stars, thin hexagons and concave octagons (solid lines) superimposed with a pentagonal modification of the Penrose tiling with rhombi (broken lines). The former tiling is a sublattice of the layer B . The edge length of the tiles is equal to the lattice constant a ($= .251$ nm). The vertices of each tile belong alternately to Q_1 or Q_2 . The latter tiling is related to the tiling Q_0 as shown in Fig. 2. The layer B decorates the two types of rhombi in simple rules. The layer A decorates differently this tiling from the layer B .

Fig. 6 A decagonal tiling obtained as a superposition of Q_0 and $\bar{Q}_0$ (broken lines). The pentagons show the same decagonal atom columns as in $\text{Al}_3\text{Mn}^{(18)}$. The simple and double circles show the 2D projection of the neighbouring layers B_2 and $\bar{B}_2$, respectively.

pentagons in $\bar{Q}_0$ (or Q_0). The pentagons in $\bar{Q}_0$ are derived from these overlapping pentagons, which yield the

decagonal atom columns in Al_3Mn and $\text{Al-Mn}^{(18)}$. The 2D density of these columns is twice as large as the den-

sity of the lattice points of Q_3 .

The two composite layers C and $\bar{C}$ neighbour through $B_2\bar{B}_2$, whose $2D$ projection, $Q_2 + \bar{Q}_2$, decorates $\bar{Q}_0$ as shown in Fig. 6. The projected $2D$ QL has short-spacing pairs of sites, which are derived from overlapping of non-pentagonal tiles of Q_0 and $\bar{Q}_0$ and partial overlapping of the pentagons.

V. Discussions and Conclusions

$\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ ⁽²⁶⁾ is a different approximant crystal to Al-Mn from Al_3Mn . It is composed of the same hexagonal tiles as those in Al_3Mn but with a different arrangement⁽²⁵⁾. A prescription of obtaining a periodic approximant with a given size and symmetry is presented in Ref. (22). Our model in this paper has not only Al_3Mn but also $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ as its approximants.

We have not distinguished the Al and Mn sites in our model QL. According to the structure of Al_3Mn ⁽¹⁸⁾, the sublattice Q_4 in the layer A is composed of Mn sites only, while other sublattices in the layer A as well as in the layer B_1 are composed of Al sites only. On the other hand, the layer B_2 ($=Q_2$) is a mixture of Al and Mn sites. The AS S_2 of Q_2 can be divided into two different sub-ASs from those in Fig. 3, i.e., one at the centre and the other being the remaining annular part, so that the sublattice derived from the central sub-AS refers to Mn sites. The chemical ordering model discussed so far is, however, not quite consistent with the structure of $\text{Al}_{60}\text{Mn}_{11}\text{Ni}_4$ ⁽²⁶⁾. It should be refined on the basis of the X-ray data on a single crystal of Al-Mn⁽⁶⁾.

The ASs used in our model QL have a common feature to those of the Burkov model⁽⁷⁾ for Al-Cu-Co: They are polygons whose edges vectors are given by $\tau^{-k}e_i'$, $i=0-4$, where k is a common integer among different ASs and represents the "order" of the ASs. The order of our ASs is two.

The model QL is consistent with the results of the X-ray analysis of Al-Mn reported by Steurer⁽⁶⁾ except that the atoms derived from Q_2' in the layer A and Q_3 in the layer B are absent in the latter result. The fraction of these atoms is about 8%. It is not known whether these atoms are retrieved by refining the analysis of the X-ray data. The sizes and forms of ASs S_0 , S_1 , S_2 and S_4 are in good agreement with the results by Steurer⁽⁶⁾.

We now compare our model with the one by Li and Kuo⁽⁹⁾ (to be referred to as L-K). L-K is based on the decagonal Penrose tiling with rhombic tiles, while our model on the generalized Penrose tiling. A detailed analysis revealed that L-K is obtained from our model by modifying the $2D$ QLs appropriately; the $2D$ QLs, $\hat{Q}_p$, $p=0-4$, in L-K have different ASs, $\hat{S}_p$, from ours. $\hat{S}_0$ is a regular decagon and $\hat{Q}_0$ the decagonal Penrose tiling introduced in Section III. The three ASs $\hat{S}_p$ with $p=2-3$ are obtained basically from our S_p by replacing their star sub-ASs by the pentagons which circumscribe them, while $\hat{S}_1 = -\hat{S}_4$. The thin hexagons in S_2 become thin rhombi in $\hat{S}_2$. The pentagonal sub-ASs of $\hat{S}_p$ are derived from decagons or stars in S_p depending on the orienta-

tions of the pentagons. The ASs in L-K are similar to polygons embedded in the decagonal Penrose tiling $\hat{Q}_0$. These ASs are identical or almost identical with those used by Edagawa *et al.*⁽⁸⁾ in their investigation of another DQC, Al-Ni-Co.

The most important feature of L-K is that $\hat{Q}_0$ includes stars and boats in the negative orientations. These tiles are decorated by the lattice points of $\hat{Q}_2$ so that the shortest spacing in the layer B is a/τ ($=.15$ nm), which is physically not allowed (see Fig. 6(c) in Li and Kuo⁽⁹⁾). The wrong site-pairs can be avoided if the thin rhombi in $\hat{S}_2$ are trimmed by the regular decagon circumscribing S_2 , the original AS. The resulting AS is, however, clumsy and this modified L-K will not be a better model than ours. We should note another point: Since the point symmetry of the sublattice L_0 in the layer A of the $3D$ QL is not decagonal but pentagonal, the use of the decagonal AS as in L-K is not necessary.

There exists the second pentagonal modification of the Penrose tiling with pentagons: It has a Burkov type AS whose order is four. We shall not, however, discuss the model QL for Al_3Mn based on this tiling.

In conclusion, there exist several structural models of Al-Mn but our model is best at present because it is simple yet has many desirable properties.

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REFERENCES

- (1) V. Kumar, D. Sahoo and G. Athithan: Phys. Rev., **B34** (1986), 6924.
- (2) A. Yamamoto and K. N. Ishihara: Acta Cryst., **A44** (1988), 707.
- (3) A. Yamamoto, K. Kato, T. Shibuya and S. Takeuchi: Phys. Rev. Lett., **65** (1990), 1603.
- (4) W. Steurer and K. H. Kuo: Acta Cryst., **B46** (1990), 703.
- (5) W. Steurer: Z. Kristallographie, **190** (1990), 179.
- (6) W. Steurer: J. Phys.: Condens. Matter, **3** (1991), 3397.
- (7) S. E. Burkov: Phys. Rev. Lett., **67** (1991), 614.
- (8) K. Edagawa, N. Naito, K. Suzuki, T. Hashimoto, S. Takeuchi and T. Shibuya: Quasicrystals, ed. K. H. Kuo and T. Ninomiya, World Scientific, Singapore, (1991), p. 56.
- (9) X. Z. Li and K. H. Kuo: Phil. Mag., **B65** (1992), 525.
- (10) X. Z. Li and K. H. Kuo: Phil. Mag. Lett., **58** (1988), 167.
- (11) T. Janssen: Phys. Rep., **168** (1988), 55.
- (12) T. Janssen: Acta Cryst., **A42** (1986), 261.
- (13) K. Niizeki: J. Phys. A: Math. Gen., **25** (1989), 205.
- (14) V. Elser: Acta Cryst., **A42** (1986), 36.
- (15) C. L. Henley: J. Non-Cryst. Solids, **75** (1985), 91.
- (16) H. Zhang and K. H. Kuo: Phys. Rev., **B42** (1990), 9807.
- (17) K. Hiraga, W. Sun and F. J. Lincoln: Jpn. J. Appl. Phys., **30** (1991), L302.
- (18) K. Hiraga, M. Kaneko, Y. Matsuo and S. Hashimoto: Phil. Mag., **B65** (1992), in press.
- (19) K. N. Ishihara and A. Yamamoto: Acta Cryst., **A44** (1988), 508.
- (20) K. Niizeki: J. Phys. A: Math. Gen., **22** (1989), 193, 4281.
- (21) K. Niizeki: J. Phys. A: Math. Gen., **23** (1990), 4569.
- (22) K. Niizeki: J. Phys. A: Math. Gen., **25** (1992), 4559.
- (23) A. Pavlovitch and M. Kléman: J. Math. Gen., **20** (1987), 687.
- (24) C. L. Henley: Phys. Rev., **B34** (1986), 797.
- (25) X. Z. Li and K. H. Kuo: Phil. Mag., **B66** (1992), 117.
- (26) A. Damjanovic: Acta Cryst., **14** (1961), 982.