

Understanding Fivefold Symmetry in Electron-Diffraction Patterns

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Abstract

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Full Text

Preamble

Understanding Fivefold Symmetry in Electron-Diffraction Patterns

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Abstract

Electron-diffraction patterns with 5-fold rotational symmetry from experimental alloy phases are assumed to be produced by periodic structures. A three-dimensional periodic structure is presented based on two types of polyhedra. The structure can be used as an orthorhombic unit cell atomic model to describe the alloy phases. The Fourier-transform patterns of the model are simulated along six “symmetry directions.” The chemical composition of the model is similar to that of the Al-Mn alloy phase. Details of the motivations and approaches

leading to these models are discussed. This study suggests that non-classical periodic structures are also viable candidates for describing quasicrystals. Further studies in this area are encouraged.

Keywords: Condensed matter physics; Electron-diffraction; 5-fold symmetry; Quasicrystal; Two kind polyhedrons; Periodic model; Fourier-transform patterns

Introduction

According to classical crystallographic theory, a crystal structure can have n -fold rotational symmetry only if $n = 2, 3, 4,$ or 6 . As a consequence, the diffraction patterns of crystal structures exhibit only these same n -fold symmetries. The discovery of alloy phases exhibiting electron-diffraction patterns (EDPs) with 5-, 8-, 10-, and 12-fold rotational symmetry consisting of sharp peaks [1, 2, 3, 4, 5] has broken this crystallographic restriction.

The prevailing view is that these alloy phases represent a fundamentally new class of ordered atomic structures exhibiting long-range quasiperiodic translational order and long-range orientational order with crystallographically forbidden symmetry, though in practice these phases may be randomly packed [6]. Such phases are called quasicrystals (QCs) [6].

EDPs showing 12-fold rotational symmetry were observed by Chen, Li, and Kuo [5] in V-Ni and V-Ni-Si alloys in 1988. The group interpreted these alloys as two-dimensional quasicrystals rather than crystals. In previous work [7, 8, 9], we introduced several three-dimensional periodic structures based on so-called T-polyhedra. These structures have been used as mathematical models to describe the V-Ni and V-Ni-Si alloy systems. The Fourier-transform patterns (FTPs) of the models were in good agreement with all the corresponding EDPs of these alloys.

In previous versions of this study [10], we reported that the high-resolution electron microscopy (HREM) image of Mn-Al-Si, taken with the incident beam parallel to the fivefold symmetry zone axis, cannot be described by Penrose tiling [see Fig. 3 [Figure 3: see original paper] in Ref. [11]]; the HREM image reported by Hiraga et al. [11] exhibits periodic characteristics formed by isolated and overlapping regular decagons [see Fig. 1 [Figure 1: see original paper]]. The positions of the spots in the EDP showing 5-fold rotational symmetry can be assumed to be located at integral lattice points in an orthogonal coordinate system. Several periodic models were proposed to interpret the HREM images and EDPs of quasicrystals with 5-fold rotational symmetry [11, 1]. After detailed study, this paper presents an updated periodic model. This model can better interpret the HREM image [11] of the fivefold QC and the EDPs [1] of the fivefold QC along six “symmetry directions.”

Figure 1: The HREM image of Mn-Al-Si QC with the incident beam along the “five-fold symmetry” axis shows periodic characteristics. Some strong bright

spots form regular dodecagons (embedded by weak bright spots) that exist in isolated or overlapped arrangements. [Courtesy of K. Hiraga, Tohoku University. Also see Fig. 2 in Ref. [11]].

Figure 2 [Figure 2: see original paper]: The tiling formed by the projection on the x-y plane of the periodic model.

The HREM image reported by Hiraga et al. [11] may be described by Fig. 2. It is formed by the projection on the x-y plane of the following fundamental units [see Figs. 3-7]: (a) Isolated and overlapping polyhedra (denoted by PPRPs), where each polyhedron has 12 pentagonal faces with regular pentagons at the top and bottom. (b) Along the z-axis direction, polyhedra with 10 triangular faces and regular pentagonal top and bottom are formed. (c) Surrounding each isolated polyhedron are two layers of regular pentagons. (d) Each isolated PPRP has ten surrounding atoms on circles centered at the PPRP (see the black dots in Figs. 2-4).

The rest of the paper is divided into three sections. Section 2 constructs the periodic mathematical model. Section 3 simulates the FTPs of the model. Finally, Sect. 4 concludes the paper.

2 Three-Dimensional Periodic Mathematical Model

The projection of the model on the x-y plane is shown in Fig. 2. In a unit cell, there are two isolated PPRPs and four overlapping PPRPs. There are 10×4 atoms + 7×4 atoms surrounding the PPRPs [see Ce1-Ce8 in Figs. 3-5].

Figure 2 is similar to the HREM image obtained by Hiraga et al. from Al-Mn-Si alloy [see Fig. 1 and Fig. 2 in Ref. [11]]. Therefore, the model is generated by orthorhombic cells.

Let r be the radius of the projection circles of the PPRPs [see Fig. 2]. The lengths of the orthorhombic cell are given as follows:

Figure 3: Three-dimensional structures of overlapping PPRPs and isolated PPRPs with surrounding atoms. Each PPRP translates by distance $|\rightarrow a3|$ along the z-axis direction, forming a polyhedron with 10 triangular faces and regular pentagonal top and bottom.

Figure 4 [Figure 4: see original paper]: The projection on the x-y plane of two overlapping PPRPs and one isolated PPRP with surrounding atoms. $|\rightarrow a1| = r(5 + 6 \sin(\pi/10))$, $|\rightarrow a2| = 4r(1 + \sin(\pi/10)) \cos(\pi/10)$, $|\rightarrow a3| = 4r$ where $a1$, $a2$ and $a3$ are primitive lattice vectors.

Figure 5 [Figure 5: see original paper]: The projection on the x-z plane of two overlapping PPRPs and one isolated PPRP with surrounding atoms.

The positions of the twenty atoms of a PPRP with center at $(0, 0, 0)$ are listed in Table 1. The positions of the four “centers” of a PPRP with center at $(0, 0, 0)$ are given in Table 2.

Table 1: The positions of the twenty atoms in a PPRP with center at $(0, 0, 0)$ where $j = 1, 2, 3, 4, 5$.

Table 2: The positions of the four “center” atoms of a PPRP with center at $(0, 0, 0)$.

Figure 6 [Figure 6: see original paper]: The three-dimensional structures of isolated PPRPs with surrounding atoms.

Each PPRP translates by $|\rightarrow a_3|$ along the z-axis direction, forming a new polyhedron with 10 triangular faces and regular pentagons on its top and bottom. The edges of the new polyhedron are the same as those of the PPRP [see Fig. 3 and Fig. 5].

Let $C_{i\hat{0}}$ ($i = 1, 2, \dots, 6$) denote the centers of the six PPRPs (see $C_{j\hat{0}}$, $j = 1, 2, \dots, 6$, in Figs. 2 and 3) in a primitive unit cell. $C_{i\hat{0}}$ have the following forms:

$$\begin{aligned} C_{1\hat{0}} &= (0, 0, 0) \\ C_{2\hat{0}} &= (r(1 + 2 \sin(\pi/10)), 0, 0) \\ C_{3\hat{0}} &= (2r(1 + \sin(\pi/10)), 0, 0) \\ C_{4\hat{0}} &= (2r(1 + \sin(\pi/10)) \cos(2\pi/5), 2r(1 + \sin(\pi/10)) \sin(2\pi/5), 0) \\ C_{5\hat{0}} &= (r(1 + 2 \sin(\pi/10)) + 2r(1 + \sin(\pi/10)), 0, 0) \\ C_{6\hat{0}} &= (2r(1 + \sin(\pi/10)) + r(1 + 2 \sin(\pi/10)), 0, 0) \end{aligned}$$

The positions of the atoms of the m-th PPRP can be denoted by:

$$C_{\{m,i\}\hat{j}} = C_{m\hat{0}} + (x_{i\hat{j}}, y_{i\hat{j}}, z_{i\hat{j}}), j = 1, 2, 3, 4, 5; i = 1, 2, 3, 4; m = 1, 2, \dots, 6.$$

The “center” positions of the atoms of the m-th PPRP can be denoted by:

$$C_{\{m,i\}\hat{0}} = C_{m\hat{0}} + (x_{i\hat{0}}, y_{i\hat{0}}, z_{i\hat{0}}), i = 1, 2, 3, 4; m = 1, 2, \dots, 6.$$

The positions of the surrounding atoms $C_{\{ei\}}$ ($i = 1, \dots, 8$) have the following forms [see Figs. 3-5]:

$$\begin{aligned} Ce_1 &= (-r(1 + 2 \sin(\pi/10)) \cos(\pi/5), -r(1 + 2 \sin(\pi/10)) \sin(\pi/5), 3r/2) \\ Ce_2 &= (r(1 + 2 \sin(\pi/10)) - x_{1e}, y_{1e}, 3r/2) \\ Ce_3 &= (x_{1e}, -y_{1e}, 3r/2) \\ Ce_4 &= (x_{2e}, -y_{1e}, 3r/2) \\ Ce_5 &= (-r(1 + 2 \sin(\pi/10)) \cos(72\pi/180), r(1 + 2 \sin(\pi/10)) \sin(72\pi/180), 3r/2) \\ Ce_6 &= (2r(1 + \sin(\pi/10)) \cos(\pi/5), 2r(1 + \sin(\pi/10)) \sin(\pi/5), 3r/2) \\ Ce_7 &= (x_{5e}, 2r(1 + \sin(\pi/10)) \sin(2\pi/5) - y_{1e}, 3r/2) \\ Ce_8 &= (x_{6e}, y_{7e}, 3r/2) \end{aligned}$$

The positions of the four atoms at e_m ($m = 1, \dots, 8$) along the z-axis direction have the forms:

$$\begin{aligned} C_{\{m,1\}\hat{e}} &= (x_{\{me\}}, y_{\{me\}}, 3r/2) \\ C_{\{m,2\}\hat{e}} &= (x_{\{me\}}, y_{\{me\}}, r/2) \end{aligned}$$

$$\begin{aligned} C_{\{m,3\}}^{\wedge e} &= (x_{\{me\}}, y_{\{me\}}, -r/2) \\ C_{\{m,4\}}^{\wedge e} &= (x_{\{me\}}, y_{\{me\}}, -3r/2) \end{aligned}$$

The vertex atoms of the regular pentagons surrounding $C_{\{5,j\}}^{e-C_{\{8,j\}}e}$ ($j = 1, 4$) can be denoted by:

$$C_{\{m,i\}}^{\wedge \{je\}} = (x_{\{me\}}, y_{\{me\}}, 0) + (x_{\{i\}}^{\wedge j}, y_{\{i\}}^{\wedge j}, z_{\{i\}}^{\wedge j})$$

Among the vertices of the regular pentagons surrounding $C_{\{1,1\}}^{e-C_{\{8,1\}}e}$, there are some that need to be deleted [see Figs. 7 and 9]. These can be described as 12 vertices overlapping or too close to the vertices of the regular pentagons surrounding $C_{\{5,1\}}^{e-C_{\{8,4\}}e}$ and $C_{\{1,4\}}^{e-C_{\{4,4\}}e}$ as follows.

Let:

$$\begin{aligned} x_{\{00\}} &= \cos(\pi/5), y_{\{00\}} = \sin(\pi/5) \\ x_{\{jb\}} &= 2 \sin(\pi/10) \cos(j\pi/5), y_{\{jb\}} = 2 \sin(\pi/10) \sin(j\pi/5), z_{\{jb\}} = \\ &(-1)^{\wedge j} 7/2, j = 0, \dots, 9 \end{aligned}$$

Then:

$$\begin{aligned} C_{\{7,i\}}^{\wedge \{je\}} &= (x_{\{7e\}} - x_{\{00\}}, y_{\{7e\}} + y_{\{00\}}, 0) + (x_{\{jb\}}, y_{\{jb\}}, \\ &z_{\{jb\}}), j = 2, 3, \dots, 8 \\ C_{\{8,i\}}^{\wedge \{je\}} &= (x_{\{8e\}} + x_{\{00\}}, y_{\{8e\}} + y_{\{00\}}, 0) + (x_{\{jb\}}, y_{\{jb\}}, \\ &z_{\{jb\}}), j = 1, 2, 3, 4, 5, 9, 10 \\ C_{\{5,i\}}^{\wedge \{je\}} &= (x_{\{5e\}} - x_{\{00\}}, y_{\{5e\}} - y_{\{00\}}, 0) + (x_{\{jb\}}, y_{\{jb\}}, \\ &z_{\{jb\}}), j = 4, 5, \dots, 10 \\ C_{\{6,i\}}^{\wedge \{je\}} &= (x_{\{6e\}} + x_{\{00\}}, y_{\{6e\}} - y_{\{00\}}, 0) + (x_{\{jb\}}, y_{\{jb\}}, \\ &z_{\{jb\}}), j = 1, 2, 3, 7, 8, 9, 10 \end{aligned}$$

Furthermore, let $r_1 = \sin(2\pi/5) + \sin(\pi/10) \tan(3\pi/10)$. The ten surrounding atoms on the circles centered at the isolated PPRPs at C3 and C4 (see the black dots in Figs. 2-4) can be described by:

$$\begin{aligned} C_{\{3,j\}}^{\wedge \{r_1\}} &= C_3^{\wedge 0} + r_1(\cos(\pi(18 + 36j)/180), \sin(\pi(18 + 36j)/180), 0), j \\ &= 0, 1, \dots, 9 \\ C_{\{4,j\}}^{\wedge \{r_1\}} &= C_4^{\wedge 0} + r_1(\cos(\pi(18 + 36j)/180), \sin(\pi(18 + 36j)/180), 0), j \\ &= 0, 1, \dots, 9 \end{aligned}$$

In summary, we construct an orthorhombic cell model. In a primitive unit cell, there are 264 atoms. The distances between two adjacent atoms in the primitive unit cell are listed as follows [see Figs. 8-9]:

$$\begin{aligned} d_1 &= 2r \sin(\pi/10) \quad 0.6180r \\ d_2 &= 4r \sin(\pi/10) \sin(\pi/5) \quad 0.7265r \\ d_3 &= r \\ d_4 &= r\sqrt{((1 - 2 \sin(\pi/10))^2 + 1)} \quad 0.9539r \\ d_5 &= r\sqrt{((4 \sin(\pi/10) + 1)(\sin(\pi/5) - \sin(2\pi/5)))^2 + (10 \cos(\pi/10)^2 - 8 \\ &\cos(\pi/10)^4 - 2)^2} \quad 1.0705r \\ d_6 &= \sin(\pi/10)(2 \sin(2\pi/5) + 2 \sin(\pi/10) \tan(3\pi/10)) \quad 0.8507r \end{aligned}$$

3.1 FTPs of the Model

Now we use the primitive lattice vectors a_1 , a_2 , and a_3 to express the coordinates of the atoms defined by (10)-(31).

- (1) For the atoms located at positions defined by (10):

$$C_{\{m,i\}^j} = \alpha_{\{m,i\}^j} a_1 + \beta_{\{m,i\}^j} a_2 + \gamma_{\{m,i\}^j} a_3$$
- (2) For the atoms located at positions defined by (11):

$$C_{\{m,i\}^0} = \alpha_{\{m,i\}^0} a_1 + \beta_{\{m,i\}^0} a_2 + \gamma_{\{m,i\}^0} a_3$$
- (3) For the atoms located at positions defined by (20)-(23):

$$C_{\{m,i\}^e} = \alpha_{\{m,i\}^e} a_1 + \beta_{\{m,i\}^e} a_2 + \gamma_{\{m,i\}^e} a_3$$
- (4) For the atoms located at positions defined by (24):

$$C_{\{m,i\}^{\{je\}}} = \alpha_{\{m,i\}^{\{je\}}} a_1 + \beta_{\{m,i\}^{\{je\}}} a_2 + \gamma_{\{m,i\}^{\{je\}}} a_3$$
- (5) For the atoms located at positions defined by (27)-(30):

$$C_{\{7,i\}^{\{je\}}} = \alpha_{1^{\{je\}}} a_1 + \beta_{1^{\{je\}}} a_2 + \gamma_{1^{\{je\}}} a_3 \text{ for } j = 2, 3, \dots, 8$$

$$C_{\{8,i\}^{\{je\}}} = \alpha_{2^{\{je\}}} a_1 + \beta_{2^{\{je\}}} a_2 + \gamma_{2^{\{je\}}} a_3 \text{ for } j = 1, 2, 3, 4, 5, 9, 10$$

$$C_{\{5,i\}^{\{je\}}} = \alpha_{3^{\{je\}}} a_1 + \beta_{3^{\{je\}}} a_2 + \gamma_{3^{\{je\}}} a_3 \text{ for } j = 4, 5, \dots, 10$$

$$C_{\{6,i\}^{\{je\}}} = \alpha_{4^{\{je\}}} a_1 + \beta_{4^{\{je\}}} a_2 + \gamma_{4^{\{je\}}} a_3 \text{ for } j = 1, 2, 3, 7, 8, 9, 10$$
- (6) For the atoms located at positions defined by (31)-(32):

$$C_{\{3,j\}^{\{r1\}}} = \alpha_{3^{\{jr1\}}} a_1 + \beta_{3^{\{jr1\}}} a_2 + \gamma_{3^{\{jr1\}}} a_3 \text{ for } 1 \leq j \leq 10$$

$$C_{\{4,j\}^{\{r1\}}} = \alpha_{4^{\{jr1\}}} a_1 + \beta_{4^{\{jr1\}}} a_2 + \gamma_{4^{\{jr1\}}} a_3 \text{ for } 1 \leq j \leq 10$$

From formulas (33)-(48), the distribution of atoms in the model may be expressed by the function:

$$\begin{aligned} (r) = & \sum_{\{h,k,l=-\infty\}^{\infty}} [\sum_{\{m,i,j\}} f_{\{ijm\}} \delta(r - (h + \alpha_{\{m,i\}^j})a_1 - (k + \beta_{\{m,i\}^j})a_2 - (l + \gamma_{\{m,i\}^j})a_3) \\ & + \sum_{\{m,i\}} f_{\{im\}} \delta(r - (h + \alpha_{\{m,i\}^0})a_1 - (k + \beta_{\{m,i\}^0})a_2 - (l + \gamma_{\{m,i\}^0})a_3) \\ & + \sum_{\{m,i\}} f_{\{emi\}} \delta(r - (h + \alpha_{\{m,i\}^e})a_1 - (k + \beta_{\{m,i\}^e})a_2 - (l + \gamma_{\{m,i\}^e})a_3) \\ & + \sum_{\{m,i,j\}} f_{\{eijm\}} \delta(r - (h + \alpha_{\{m,i\}^{\{je\}}})a_1 - (k + \beta_{\{m,i\}^{\{je\}}})a_2 - (l + \gamma_{\{m,i\}^{\{je\}}})a_3) \\ & + \sum_{\{j=2,3,\dots,8\}} f_{\{1ej\}} \delta(r - (h + \alpha_{1^{\{je\}}})a_1 - (k + \beta_{1^{\{je\}}})a_2 - (l + \gamma_{1^{\{je\}}})a_3) \\ & + \sum_{\{j=1,2,3,4,5,9,10\}} f_{\{2ej\}} \delta(r - (h + \alpha_{2^{\{je\}}})a_1 - (k + \beta_{2^{\{je\}}})a_2 - (l + \gamma_{2^{\{je\}}})a_3) \\ & + \sum_{\{j=4,5,\dots,10\}} f_{\{3ej\}} \delta(r - (h + \alpha_{3^{\{je\}}})a_1 - (k + \beta_{3^{\{je\}}})a_2 - (l + \gamma_{3^{\{je\}}})a_3) \end{aligned}$$

$$\begin{aligned}
& + \sum_{\{j=1,2,3,7,8,9,10\}} f_{\{4ej\}} \delta(r - (h + \alpha_{-4}^{\{je\}})a_1 - (k + \beta_4^{\{je\}})a_2 - (l + \gamma_4^{\{je\}})a_3) \\
& + \sum_{\{j=1\}^{\{10\}}} f_{\{3jr1\}} \delta(r - (h + \alpha_{-3}^{\{jr1\}})a_1 - (k + \beta_3^{\{jr1\}})a_2 - (l + \gamma_3^{\{jr1\}})a_3) \\
& + \sum_{\{j=1\}^{\{10\}}} f_{\{4jr1\}} \delta(r - (h + \alpha_{-4}^{\{jr1\}})a_1 - (k + \beta_{-4}^{\{jr1\}})a_2 - (l + \gamma_{-4}^{\{jr1\}})a_3)]
\end{aligned}$$

where $f_{\{ijm\}}$, $f_{\{im\}}$, $f_{\{emi\}}$, $f_{\{eijm\}}$, $f_{\{1ej\}}$, $f_{\{2ej\}}$, $f_{\{3ej\}}$, $f_{\{4ej\}}$, $f_{\{3jr1\}}$, and $f_{\{4jr1\}}$ are the scattering factors of the atoms at positions $C_{\{m,i\}}^{\{j\}}$, $C_{\{m,i\}}^0$, $C_{\{m,i\}}^e$, $C_{\{m,i\}}^{\{je\}}$, $C_{\{1,i\}}^{\{je\}}$, $C_{\{2,i\}}^{\{je\}}$, $C_{\{3,i\}}^{\{je\}}$, $C_{\{4,i\}}^{\{je\}}$, $C_{\{3,j\}}^{\{r1\}}$, and $C_{\{4,j\}}^{\{r1\}}$, respectively. For simplicity, we set all scattering factors equal to one.

The diffraction intensity $I(h, k, l)$ (Fourier-transform pattern) at the reciprocal-lattice point $ha_1 + ka_2 + la_3$ is given by:

$$I(h, k, l) = \int_V |\exp(-i(ha_1 + ka_2 + la_3) \cdot r)|^2 dx dy dz$$

where V is a constant. Therefore:

$$\begin{aligned}
I(h, k, l) = & [(\sum f_{\{ijm\}} \cos(2\pi(h\alpha_{\{m,i\}}^{\{j\}} + k\beta_{\{m,i\}}^{\{j\}} + l\gamma_{\{m,i\}}^{\{j\}})) + \sum f_{\{im\}} \cos(2\pi(h\alpha_{\{m,i\}}^0 + k\beta_{\{m,i\}}^0 + l\gamma_{\{m,i\}}^0)) \\
& + \sum f_{\{emi\}} \cos(2\pi(h\alpha_{\{m,i\}}^e + k\beta_{\{m,i\}}^e + l\gamma_{\{m,i\}}^e)) + \sum f_{\{eijm\}} \cos(2\pi(h\alpha_{\{m,i\}}^{\{je\}} + k\beta_{\{m,i\}}^{\{je\}} + l\gamma_{\{m,i\}}^{\{je\}})) \\
& + \sum_{\{j=2,\dots,8\}} f_{\{1ej\}} \cos(2\pi(h\alpha_1^{\{je\}} + k\beta_1^{\{je\}} + l\gamma_1^{\{je\}})) + \sum_{\{j=1,2,3,4,5,9,10\}} f_{\{2ej\}} \cos(2\pi(h\alpha_2^{\{je\}} + k\beta_2^{\{je\}} + l\gamma_2^{\{je\}})) \\
& + \sum_{\{j=4,\dots,10\}} f_{\{3ej\}} \cos(2\pi(h\alpha_3^{\{je\}} + k\beta_3^{\{je\}} + l\gamma_3^{\{je\}})) + \sum_{\{j=1,2,3,7,8,9,10\}} f_{\{4ej\}} \cos(2\pi(h\alpha_4^{\{je\}} + k\beta_4^{\{je\}} + l\gamma_4^{\{je\}})) \\
& + \sum_{\{j=1\}^{\{10\}}} f_{\{3jr1\}} \cos(2\pi(h\alpha_3^{\{jr1\}} + k\beta_3^{\{jr1\}} + l\gamma_3^{\{jr1\}})) + \sum_{\{j=1\}^{\{10\}}} f_{\{4jr1\}} \cos(2\pi(h\alpha_4^{\{jr1\}} + k\beta_4^{\{jr1\}} + l\gamma_4^{\{jr1\}}))]^2 \\
& + (\sum f_{\{ijm\}} \sin(2\pi(h\alpha_{\{m,i\}}^{\{j\}} + k\beta_{\{m,i\}}^{\{j\}} + l\gamma_{\{m,i\}}^{\{j\}})) + \sum f_{\{im\}} \sin(2\pi(h\alpha_{\{m,i\}}^0 + k\beta_{\{m,i\}}^0 + l\gamma_{\{m,i\}}^0)) \\
& + \sum f_{\{emi\}} \sin(2\pi(h\alpha_{\{m,i\}}^e + k\beta_{\{m,i\}}^e + l\gamma_{\{m,i\}}^e)) + \sum f_{\{eijm\}} \sin(2\pi(h\alpha_{\{m,i\}}^{\{je\}} + k\beta_{\{m,i\}}^{\{je\}} + l\gamma_{\{m,i\}}^{\{je\}})) \\
& + \sum_{\{j=2,\dots,8\}} f_{\{1ej\}} \sin(2\pi(h\alpha_1^{\{je\}} + k\beta_1^{\{je\}} + l\gamma_1^{\{je\}})) + \sum_{\{j=1,2,3,4,5,9,10\}} f_{\{2ej\}} \sin(2\pi(h\alpha_2^{\{je\}} + k\beta_2^{\{je\}} + l\gamma_2^{\{je\}})) \\
& + \sum_{\{j=4,\dots,10\}} f_{\{3ej\}} \sin(2\pi(h\alpha_3^{\{je\}} + k\beta_3^{\{je\}} + l\gamma_3^{\{je\}})) + \sum_{\{j=1,2,3,7,8,9,10\}} f_{\{4ej\}} \sin(2\pi(h\alpha_4^{\{je\}} + k\beta_4^{\{je\}} + l\gamma_4^{\{je\}})) \\
& + \sum_{\{j=1\}^{\{10\}}} f_{\{3jr1\}} \sin(2\pi(h\alpha_3^{\{jr1\}} + k\beta_3^{\{jr1\}} + l\gamma_3^{\{jr1\}})) + \sum_{\{j=1\}^{\{10\}}} f_{\{4jr1\}} \sin(2\pi(h\alpha_4^{\{jr1\}} + k\beta_4^{\{jr1\}} + l\gamma_4^{\{jr1\}})))^2]
\end{aligned}$$

where we set $V = 0.001$.

The FTPs of the model along different “symmetry directions” are shown in Figs. 10, 12–15. The FTP diffraction spots are shown as circles whose diameters are proportional to their intensities; spots with intensities less than $0.08I(0, 0, 0)$ are omitted.

Figure 11 [Figure 11: see original paper] shows a typical EDP of a quasicrystal with fivefold rotational symmetry [12].

The FTPs shown in Figs. 10 and 12 are very similar to the corresponding QC EDPs [see Fig. 11, or Fig. 2 in Ref. [1]]. The FTPs shown in Figs. 13-16 have characteristics corresponding to the QC EDPs [see Fig. 2 in Ref. [1]]. The positions of the line-connected spots shown in Figs. 13-16 are in good agreement with the positions of the corresponding strong spots shown in Fig. 2 of Ref. [1].

In addition, if we let $r = 6.5 \text{ \AA}$, then the volume of the primitive unit cell of the model is $44.5517 \times 32.3687 \times 26 \text{ \AA}^3$. Formulas (33)-(38) show that the interatomic distances of the model are between $d_{\{\min\}} = 2r \sin(\pi/10) = 4.017 \text{ \AA}$ and $d_{\{\max\}} = r\sqrt{(1 - 2 \sin(\pi/10))^2 + 1} = 6.8512 \text{ \AA}$.

Furthermore, if Al atoms occupy the vertex positions of the regular pentagons surrounding $C_{\{5,j\}}^{e-C_{\{8,j\}}e}$ ($j = 1, 4$) [see formula (24) and Fig. 6] in a primitive unit cell, and Mn atoms occupy the other positions, then there are 40 Al atoms and 224 Mn atoms in a primitive unit cell. Hence the chemical composition of the model is about $\text{Al}_{15}\text{Mn}_{85}$, which is very close to the chemical composition of fivefold rotational symmetry quasicrystals [1]. Therefore, the atomic structure presented here is acceptable.

In summary, the presented periodic model can generate Fourier-transform patterns similar to the corresponding EDPs of “5-fold symmetry” quasicrystals. The chemical composition of the model is very close to that of fivefold rotational symmetry quasicrystals [1].

3.2 Discussions

If the idealized EDPs of “5-fold symmetry” quasicrystals have 5-fold symmetry in a strict mathematical sense, then we can conclude that the HREM images of the quasicrystal imply that quasicrystals are perturbed quasiperiodic structures.

However, we can also reasonably assume that the diffraction spots in the idealized EDPs of “5-fold symmetry” quasicrystals are located at corresponding integral lattice points in orthogonal coordinate systems [see Figs. 6, 9 and 14], which are hardly distinguishable from a pattern with 5-fold symmetry in the strict sense. This means that “5-fold symmetry” quasicrystals are essentially crystals but do not belong to classical crystallographic space groups because none of the diffraction patterns of space groups has approximate “5-fold” symmetry. In this case, we can conclude that the HREM images of “5-fold symmetry” quasicrystals are perturbed non-classical crystals.

We prefer the second interpretation since it aligns with the widely held assumption in crystallography and solid-state physics—that pure solids are either crystalline or glassy.

4 Conclusions

Penrose patterns are widely used to describe 5-fold quasicrystals. However, they cannot describe the HREM image [Figure 18: see original paper] of the

Al-Mn-Si 5-fold quasicrystal reported by Hiraga et al. [11]. This study presents a periodic mathematical model. The projections [Figure 2: see original paper] of the model on the x-y plane can better describe the HREM image reported by Hiraga et al. [11] than Penrose patterns. The FTPs and chemical composition of our model are also close to those of the corresponding 5-fold quasicrystals [1].

Let N denote a three-dimensional lattice point set and let the infimum of the distances between two neighboring lattice points in N be larger than zero. Then for any sufficiently small positive number ϵ , we can construct an orthogonal (or oblique) coordinate system A such that for any lattice point (x, y, z) in N , there exists an integral lattice point (h, k, l) in A satisfying the condition that the distance between (x, y, z) and (h, k, l) is less than ϵ . This fact allows us to believe that the EDPs with fivefold, eightfold, tenfold, and twelfold symmetries [1, 2, 3, 4, 5] are produced by periodic structures [8]. Non-classical periodic structures are also viable candidates for describing quasicrystals. The research conducted in this paper shows promising results, and further studies in this area are encouraged.

Figure 10 [Figure 10: see original paper]: Fourier-transform pattern of the model in a plane orthogonal to a “5-fold symmetry axis” .

Figure 11: The digitized EDP of a quasicrystal with 5-fold rotational symmetry.

Figure 12 [Figure 12: see original paper]: Fourier-transform of the new model in a plane orthogonal to a “5-fold axis” with an angle 63.43° to the z-axis.

Figure 13 [Figure 13: see original paper]: Fourier-transform of the new model in a plane orthogonal to a “2-fold axis” with an angle 31.72° to the z-axis.

Figure 14 [Figure 14: see original paper]: Fourier-transform of the new model in a plane orthogonal to a “3-fold axis” with an angle 37.38° to the z-axis.

Figure 15 [Figure 15: see original paper]: Fourier-transform of the new model in a plane orthogonal to a “2-fold axis” with an angle 58.29° to the z-axis.

Figure 16 [Figure 16: see original paper]: Fourier-transform of the new model in a plane orthogonal to a “3-fold axis” with an angle 63.43° to the z-axis.

Figure 17 [Figure 17: see original paper]: The distributions of the centers of some FTP circles in Fig. 7 show almost perfect 5-fold rotational symmetry.

Figure 18 [Figure 18: see original paper]: A part of Fig. 1, in which some strong bright spots are connected with white lines, showing a Penrose pattern [Courtesy of K. Hiraga, Tohoku University].

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