

Six-dimensional crystal-structure model for i -(Al-Mn-Si) and α -(Al-Mn-Si)

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A six-dimensional (6D) crystal-structure model has been constructed for the icosahedral quasicrystal i -(Al-Mn-Si). The positions of the 6D hypercubic atoms are determined from the atomic coordinates of α -(Al-Mn-Si). There are 38 atoms in the 6D unit cell, and the number of inequivalent atoms is 4: One Mn atom is located at the origin, one (Al,Si) atom at the body center, and six (Al,Si) atoms at edge centers; the remaining 30 (Al,Si) atoms are distributed along the 15 face diagonals, and every two atoms divide a diagonal in the ratios $\tau^{-2}:\tau^{-3}:\tau^{-2}$, where $\tau \equiv (1+\sqrt{5})/2$. The 6D space group is $Pm\bar{3}5$. The projection of the 6D crystal onto the physical space with a rational (1/1) strip gives α -(Al-Mn-Si), and the projection with an irrational ($\tau/1$) strip gives i -(Al-Mn-Si). The idealized projection windows for obtaining i -(Al-Mn-Si) are polyhedra given by considering the similarity between the local atomic arrangements of i -(Al-Mn-Si) and those of α -(Al-Mn-Si) and also between the local environments of three-dimensional Penrose tiling and those of a rhombic tiling for the body-centered-cubic structure. The chemical composition and mass density of the obtained i -(Al-Mn-Si) quasicrystals have been calculated with the idealized projection windows. Electron diffraction patterns simulated with the approximate projection windows have been compared with the experimental patterns of i -(Al-Mn).

I. INTRODUCTION

The structure of icosahedral quasicrystal i -(Al-Mn-Si) is similar to that of icosahedral quasicrystal i -(Al-Mn), but the former is more nearly perfect in crystallinity.¹ Many papers dealing with their structures have been published.²⁻¹² i -(Al-Mn-Si) coexists with the crystalline phase α -(Al-Mn-Si) and is close to the latter in composition and local atomic arrangements.^{13,14} The quasicrystal structure can be described by a three-dimensional (3D) atomic decoration. It was suggested that both α -(Al-Mn-Si) and i -(Al-Mn-Si) consist of Mackay icosahedra (MI's),¹⁵ but packed in a bcc lattice and a 3D Penrose lattice respectively.^{2,4,7} A theoretical structure model of i -(Al-Mn-Si) was built from two kinds of icosahedral building block: MI and double MI (which is similar to the MI but is τ times larger).⁶ [$\tau \equiv (1+\sqrt{5})/2$.] These blocks share atoms and overlap with each other.

The quasicrystal structure can also be obtained on the basis of a six-dimensional atomic decoration.^{7,10,12,16} Some structural models were obtained based on the cut method.^{7,10,12} A structural model in 6D space for Al-Mn quasicrystals was constructed⁷ by a qualitative analysis of x-ray- and neutron-diffraction data. The corresponding 3D structure consists of MI's located at 12-fold vertices of the 3D Penrose quasilattice and the linking atoms joining MI's.⁷ A 6D structural model showing good mass density and chemical composition was proposed on the basis of the 3D and 6D Patterson analyses of α -(Al-Mn-Si) and i -(Al-Mn-Si).¹⁰ According to this model, there are only incomplete MI's in the 3D structure and a few anomalously short bonds exist because of the assumption of spherical atomic surfaces. It has been shown that a large number of MI's can be present and the unphysical short bonds can be avoided by introducing polyhedral atomic surfaces instead of spherical ones.^{11,12} In this case, although the distribution of MI's and linking atoms is reasonable, in some places the local atomic arrange-

ment appears to be different from that in α -(Al-Mn-Si).

Another approach to 6D atomic decoration is based on the projection method. In this case the atomic coordinates in the 6D unit cell can be derived from the crystal-line approximant by using a formula¹⁶ that is generally applicable to those icosahedral quasicrystals which are accompanied with a bcc or an almost bcc crystalline approximant. By using this method, a 6D hypercubic crystal-structure model for icosahedral $T2$ -phase Al_6CuLi_3 and bcc R -phase Al_5CuLi_3 has been constructed.¹⁶ The positions of 6D hypercubic-crystal-lattice atoms were determined from the atomic coordinates of the R phase. Because the 3D structure in pseudospace is arbitrary, the construction of a 6D crystal-structure model suffers from a multisolution problem. It was solved by assigning a special solution based on the rhombic tiling of the R phase. A 6D Al-Cu-Li structure model with 27 atoms inside the 6D unit cell was obtained, where all 6D hypercubic-crystal-lattice atoms are separated individually. The projection of the obtained 6D crystal structure onto the physical space with a rational (1/1) projection strip gives the structure of the R phase, and the projection with an irrational ($\tau/1$) projection strip gives the structure of the $T2$ phase. In the present paper, the same method is applied to the construction of a 6D Al-Mn-Si crystal-structure model for both i -(Al-Mn-Si) and α -(Al-Mn-Si). This model has been derived from the crystal structure of α -(Al-Mn-Si). The projection of the 6D crystal with irrational and rational projection strips gives the structures of i -(Al-Mn-Si) and α -(Al-Mn-Si), respectively.

II. IDEALIZED ATOMIC POSITIONS IN RHOMBIC TILING OF α -(Al-Mn-Si)

α -(Al-Mn-Si) with the idealized composition $(Al,Si)_{114}Mn_{24}$ belongs to the cubic crystal system. Its space group is $Pm\bar{3}$, and the lattice constant is 12.68 Å.¹⁷

There are 138 atoms in the unit cell. The crystal structure is almost body centered. The main departure from this pattern is the aluminum atom Al(3) (see Table I), which has no body-centered counterpart. This results in different coordination polyhedra around the two types of magnesium atoms Mn(1) and Mn(2).

The structure of α -(Al-Mn-Si) can be decorated in the bcc rhombic tiling by slightly shifting the atoms.² The bcc unit cell is constructed from eight prolate rhombohedra (PR) and six rhombic dodecahedra (RD), and each RD consists of two PR and two oblate rhombohedra (OR).^{2,3} All atoms are located at special positions of the PR and RD as given in Table I and shown in Fig. 1 (some of the special positions are different from those of Ref. 2). There are altogether four kinds of atomic site: a Mn site and three kinds of (Al,Si) site. Mn atoms [Mn(1,2) in Ref. 17] are located at vertices of the PR [Fig. 1(a)] and RD [Fig. 1(b)]. But not all vertices of the PR and RD are occupied. The two exterior vertices on the long body diagonal of the RD [Fig. 1(b)] and the interior vertex of the RD are not occupied by Mn atoms [Fig. 1(c)]. The empty vertices are called "type-1 vacancies." The edge centers which join an exterior type-1 vacancy of the RD to a Mn vertex are occupied by (Al,Si)-I [Al(4,5) in Ref. 17 or Al(α) in Ref. 2] atoms [Figs. 1(a) and 1(b)]. Other edge centers are empty and are called "type-2 vacancies." (Al,Si)-II [Al(1,2,6,7,8,9) in Ref. 17 or Al(β, γ) in Ref. 2] atoms occupy the positions in the long face diagonals of rhombuses which form the PR and OR. Every two (Al,Si)-II atoms divide the diagonal in the ratios $\tau^{-2}:\tau^{-3}:\tau^{-2}$ when all the four vertices of the face are occupied by Mn atoms [Fig. 1(b)]; a single (Al,Si)-II atom divides the long diagonal from the type-1 vacancy to a Mn atom in the ratio $\tau^{-1}:\tau^{-2}$ when one of face vertices is empty [Figs. 1(a) and 1(b)]. Besides, there are two more (Al,Si)-II atoms located inside the RD [Fig. 1(c)]. Their position can also be treated as the face diagonal sites if the rhombuses inside the RD are taken into consideration. Because the RD can be tiled in two different ways and the two tilings are related by a symmetry with respect to the symmetry plane orthogonal to the long diagonal of the RD,²² the (Al,Si)-II atom at the interior vertex of the RD in one way is also situated on the interior

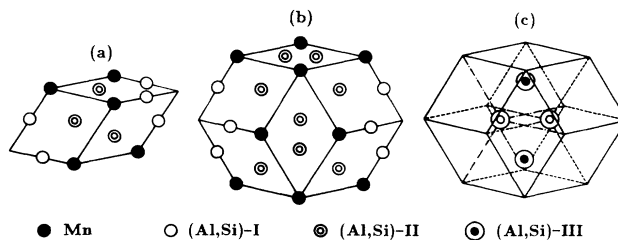


FIG. 1. Atomic decoration of idealized α -(Al-Mn-Si) in the rhombic tiling of bcc structure. There are four kinds of special positions: Mn vertices, (Al,Si)-I edge centers, (Al,Si)-II rhombic face diagonals, and (Al,Si)-III long body diagonals of a PR inside a RD. (a) Probate rhombohedron. (b) and (c) show the outer and inner view of the RD, respectively.

rhombic face diagonal in the other way and divide it in the ratio $\tau^{-1}:\tau^{-2}$ [Fig. 1(c)]. The unoccupied positions in the long diagonals are called "type-3 vacancies." The (Al,Si)-III [Al(3) in Ref. 17 or Al(δ) in Ref. 2] atom is inside the RD in one of the body-centered sublattices. This site is on the long body diagonal of a PR inside a RD and divides the diagonal in the ratio of $\tau^{-1}:\tau^{-2}$ [Figs. 1(c) and 2(b)]. The unoccupied sites on the long body diagonals of the PR are called "type-4 vacancies." In the real crystal structure of α -(Al-Mn-Si), the site which is inside another sublattice and equivalent to the position of an (Al,Si)-III atom is empty. For convenience, it is assumed to be occupied also by an (Al,Si)-III atom. In this case the idealized α -(Al-Mn-Si) is a perfect body-centered-cubic lattice. The calculated chemical composition and density are (Al,Si)₅Mn and 3.72 g cm⁻³, respectively. It should be noted that the atomic decoration in a PR outside a RD [Fig. 2(a)] is different from that inside a RD [Fig. 2(b)]. One of the differences is in the occupation of vertices by Mn atoms. This results in a different occupation of the face diagonals by (Al,Si)-II atoms. The second difference is in the occupation of the long body diagonal which is occupied by an (Al,Si)-III atom in a PR inside a RD [Fig. 2(b)], while it is empty in a PR outside a RD [Fig. 2(a)]. The third difference is that one of the vertices of a PR inside a RD (the interior vertex), which is shared with two

TABLE I. Idealized atomic coordinates in α -(Al-Mn-Si) and corresponding positions in PR and OR.

Equivalent positions	Atom		Idealized coordinates			Positions in PR or OR	Kind of atoms
	(Ref. 17)	Atoms (Ref. 2)	x	y	z		
12j	Mn(1)	Mn	$\frac{1}{2}\tau^{-1}$	0	$\frac{1}{2}\tau^{-2}$	vertex	Mn
12k	Mn(2)	Mn	$\frac{1}{2}\tau^{-2}$	$\frac{1}{2}$	$\frac{1}{2}\tau^{-1}$	vertex	Mn
6e	Al(1)	Al(β)	τ^{-2}	0	0	long face diagonal	(Al,Si)-II
6h	Al(2)	Al(β)	$\frac{1}{2}\tau^{-3}$	$\frac{1}{2}$	$\frac{1}{2}$	long face diagonal	(Al,Si)-II
6g	Al(3)	Al(δ)	$\frac{1}{2}\tau^{-1}$	$\frac{1}{2}$	0	inside RD	(Al,Si)-III
12j	Al(4)	Al(α)	$\frac{1}{4}\tau^{-1}$	0	$\frac{1}{4}\tau^{-2}$	edge center	(Al,Si)-I
12k	Al(5)	Al(α)	$\frac{1}{4}(2-\tau^{-1})$	$\frac{1}{2}$	$\frac{1}{4}\tau$	edge center	(Al,Si)-I
12j	Al(6)	Al(γ)	$\frac{1}{2}\tau^{-1}$	0	$\frac{1}{2}(2\tau-1)\tau^{-2}$	long face diagonal	(Al,Si)-II
12k	Al(7)	Al(γ)	$\frac{1}{2}\tau^{-3}$	$\frac{1}{2}$	$\frac{1}{2}\tau^{-3}$	long face diagonal	(Al,Si)-II
24l	Al(8)	Al(β)	$\frac{1}{2}\tau^{-3}$	$\frac{1}{2}\tau^{-1}$	$\frac{1}{2}\tau^{-2}$	long face diagonal	(Al,Si)-II
24l	Al(9)	Al(β)	τ^{-2}	$\frac{1}{2}\tau^{-2}$	$\frac{1}{2}\tau^{-1}$	long face diagonal	(Al,Si)-II

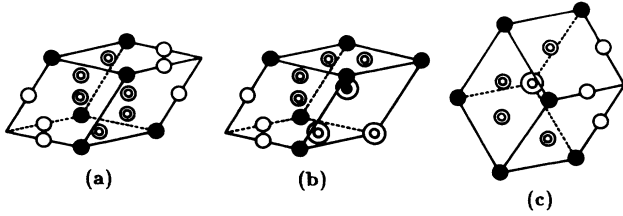


FIG. 2. Atomic decoration in a PR (a) outside a RD and (b) inside a RD. (c) Atomic decoration of the OR.

OR and another PR, is occupied by an (Al,Si)-II atom [Figs. 2(b) and 1(c)], while no (Al,Si)-II atom is located at the vertex of a PR outside a RD [Fig. 2(a)]. The atomic decoration in the OR is shown in Fig. 2(c). One of the vertices, which is shared with another OR and two PR in a RD, is occupied by an (Al,Si)-II atom instead of a Mn atom.

III. 6D CRYSTAL-STRUCTURE MODEL

The atomic coordinates of a 6D (Al-Mn-Si) hypercubic crystal structure ($x_1, x_2, x_3, x_4, x_5, x_6$) have been determined from the equation given in Ref. 16 as follows:

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix} = \frac{1}{2\tau^2} \begin{pmatrix} \tau & 0 & 1 & -1 & 0 & \tau \\ \tau & 0 & -1 & -1 & 0 & -\tau \\ 0 & 1 & -\tau & 0 & \tau & 1 \\ -1 & \tau & 0 & -\tau & -1 & 0 \\ 0 & 1 & \tau & 0 & \tau & -1 \\ 1 & \tau & 0 & \tau & -1 & 0 \end{pmatrix} \begin{pmatrix} x_{\parallel} \\ y_{\parallel} \\ z_{\parallel} \\ x_{\perp} \\ y_{\perp} \\ z_{\perp} \end{pmatrix}, \quad (1)$$

where x_{\parallel} , y_{\parallel} , and z_{\parallel} denote the atomic coordinates of α -(Al-Mn-Si). The multiresolution problem of Eq. (1) is solved by the same way as before, namely, by defining a fictitious 3D structure in pseudospace such that all vertices of the PR and OR in α -(Al-Mn-Si) correspond to vertices of the 6D hypercubic crystal lattice, etc.

After performing a coordinate transformation by using Eq. (1), positions of Mn atoms and type-1 vacancies in α -(Al-Mn-Si) are transferred to vertices in a 6D unit cell, (Al,Si)-I and type-2 vacancies to edge centers, (Al,Si)-II and type-3 vacancies to positions on face diagonals, and (Al,Si)-III and type-4 vacancies to centers in a 6D unit cell (Table II). The 6D translational symmetry constrains the 6D unit cell to have 38 atoms: 1 Mn atom at the vertex, 6 (Al,Si) atoms at edge centers, 30 (Al,Si) atoms on

face diagonals, and 1 (Al,Si) atom at the body center. Among the 30 face diagonals of the 6D unit cell, only one-half of them is occupied, and they are parallel to the directions $[110\ 000]$, $[011\ 000]$, $[001\ 100]$, $[000\ 110]$, $[100\ 010]$, $[100\ 001]$, $[010\ 001]$, $[001\ 001]$, $[000\ 101]$, $[000\ 011]$, $[10\bar{1}\ 000]$, $[010\ \bar{1}00]$, $[001\ 0\bar{1}0]$, $[\bar{1}00\ 100]$, and $[0\bar{1}0\ 010]$, respectively. Every 2 (Al,Si) atoms divide a face diagonal in the ratios $\tau^{-2}:\tau^{-3}:\tau^{-2}$. The number of inequivalent atoms is 4. The space group is $Pm\bar{3}5$.¹⁸ The lattice constant of the 6D crystal structure is 6.51 Å.

IV. FROM THE 6D CRYSTAL-STRUCTURE MODEL TO α -(Al-Mn-Si)

Because the projection of the obtained 6D crystal with (1/1) projection strip should give the idealized α -(Al-Mn-Si), 6D hypercubic-crystal-lattice atoms which originate from atoms of α -(Al-Mn-Si) should fall inside the projection strip, while those which originate from vacancies should fall outside the strip.

It is well known that the standard ($\tau/1$) projection strip which is used for obtaining the standard 3D Penrose¹⁹ tiling (3DPT) leads to a standard ($\tau/1$) projection window in pseudospace, which is a unit triacontahedron.²¹ The standard (1/1) projection strip which is obtained by rotating the standard ($\tau/1$) projection strip corresponds to a standard (1/1) projection window in pseudospace, which is a unit cubooctahedron.²⁰ The projection of the 6D hypercubic crystal lattice with the standard (1/1) strip leads to the rhombic tiling of a bcc lattice. However, with this strip the structure obtained from the projection of the above-mentioned 6D crystal structure is different from that of α -(Al-Mn-Si), because in this case the positions of the vacancies in α -(Al-Mn-Si) will in fact be occupied by atoms. In order to make the projection of the 6D crystal fit the structure of α -(Al-Mn-Si), each kind of 6D hypercubic-crystal-lattice atoms should have its own projection window. This is equivalent to the requirement that each kind of 6D hypercubic-crystal-lattice atoms has its own shape in the cut description.

If all the vacancies in rhombic tiling of α -(Al-Mn-Si) structure are transferred to the corresponding positions in the 6D crystal lattice and then to the corresponding positions in pseudospace, it could be seen that those vacancies which correspond to the same local atomic arrangement in α -(Al-Mn-Si) would be mapped to the same position in pseudospace. Hence the projection window for a certain kind of atom in α -(Al-Mn-Si) can be easily

TABLE II. Atomic coordinates in the 6D crystal-structure model.

Number of equivalent positions	Atoms	Atomic coordinates						Corresponding sites in α -(Al-Mn-Si)
		x_1	x_2	x_3	x_4	x_5	x_6	
1	Mn	0	0	0	0	0	0	Mn, type-1 vacancy
6	Al,Si	$\frac{1}{2}$	0	0	0	0	0	(Al,Si)-I, type-2 vacancy
30	Al,Si	τ^{-2}	τ^{-2}	0	0	0	0	(Al,Si)-II, type-3 vacancy
1	Al,Si	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	(Al,Si)-III, type-4 vacancy

obtained by excluding those individual positions corresponding to vacancies from the standard (1/1) projection window.

V. FROM THE 6D CRYSTAL-STRUCTURE MODEL TO i -(Al-Mn-Si)

A. Idealized projection windows

The projection of the obtained 6D crystal structure with the $(\tau/1)$ projection strip should give i -(Al-Mn-Si). However, the irrationality of the $(\tau/1)$ projection strip makes atoms and vacancies corresponding to the same local atomic arrangement be transferred to different positions in pseudospace²¹; these positions are distributed in a certain region called "an existence domain." Hence the projection window for each kind of atom can be obtained by excluding the existence domains of the corresponding vacancies from the total existence domain for both atoms and vacancies. The practical consideration of projection windows is based on the similarity between the local atomic arrangement of i -(Al-Mn-Si) and that of α -(Al-Mn-Si), and between the local environment of the 3DPT and that of rhombic tiling for bcc structure as follows.

1. Mn atoms

As mentioned in Sec. II, in the rhombic decoration of α -(Al-Mn-Si), two exterior vertices and one interior vertex of the RD are not occupied by Mn atoms. The two exterior vertices of the RD are the centers of MI's, which just correspond to the 12-fold vertices linking 12 edges in the 3DPT. The corresponding existence domain is a rhombic tricontahedron which is smaller than the unit tricontahedron by a factor τ^{-2} [Fig. 3(a)].^{7,21} According to Refs. 7 and 21, tips of the small tricontahedron along fivefold axes should be truncated to avoid the anomalous distance between MI's and the overlapping between two MI's. The truncated portion is τ^{-5} of the unit tricontahedron.^{7,21} The shape of the existence domains is shown in Fig. 3(b). The volume ratio of it to the unit tricontahedron is 0.0507.

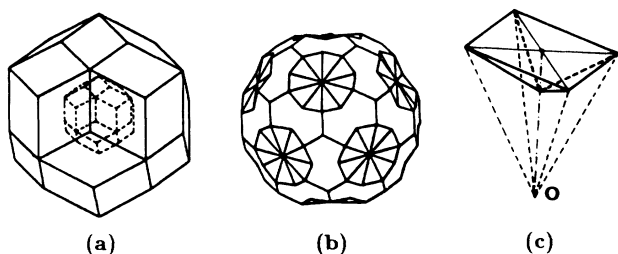


FIG. 3. (a) Unit tricontahedron (solid line), which is projection window of a standard 3DPT, and existence domain of 12-fold vertices in 3DPT (dashed line), which is also a tricontahedron, but linearly smaller by a factor τ^2 . (b) The existence domain of MI's centers, which is obtained from the existence domain of the 12-fold vertices by truncating a tip on the 5-fold axis (Ref. 21). (c) The bold lines show the existence domain of interior vertices of the RD, which is a pyramid with one of the rhombuses forming the unit tricontahedron as its base. The thin dashed lines originate from the origin in pseudospace.

The existence domain of the interior vertex of the RD is a pyramid.²¹ Its height is $\tau^{-3}A/2$. Here, A is a lattice constant of α -(Al-Mn-Si). Its base is one of the rhombuses which form the unit tricontahedron [Fig. 3(c)]. Because there are altogether 30 differently oriented RD in the standard 3DPT, the existence domain corresponding to interior vertices of all the RD consists of 30 rhombic pyramids which distribute over 30 rhombuses of the unit tricontahedron and point toward the center of it [Fig. 3(c)]. Its volume ratio to the unit tricontahedron is τ^{-3} .²¹

Therefore the projection window of Mn atoms is the residual part of the unit tricontahedron after removing from it the existence domains of exterior and interior vertices of the RD. Its volume ratio is 0.7132.

2. (Al,Si)-I atoms

In general, the existence domain of an edge formed by the basic vector e_1 in the physical space is a rhombic icosahedron²² with its center at the position $(\frac{1}{2}00000)_1$ in pseudospace, which is equivalent to the projection of a 5D hypercubic unit cell onto pseudospace formed by all other five basis vectors except the discussed one. In the atomic decoration of α -(Al-Mn-Si), (Al,Si)-I atoms occupy only the edge centers linking the centers of MI's. In this case, the existence domain of the edge center should have the same shape and size as that of centers of MI's and is placed at $(\frac{1}{2}00000)_1$. Obviously, the existence domain of the edge center for (Al,Si)-I is included in the rhombic icosahedron domain. Because 1 MI center links 12 edges, there are altogether 12 edge-center domains distributed around the origin in pseudospace. The total volume ratio of projection window to the unit tricontahedron is 12×0.0507 , or 0.6084.

3. (Al,Si)-II atoms

(Al,Si)-II atoms occupy two positions on the long face diagonal of rhombuses and divide it in the ratios $\tau^{-2}:\tau^{-3}:\tau^{-2}$. The existence domains of the rhombus formed by two basic vectors e_1, e_2 in 3DPT is a rhombic dodecahedron RD in pseudospace denoted as $(RD)_1$,²² with its center at the positions $(\frac{1}{2}\frac{1}{2}00000)_1$. It is equivalent to the projection of a 4D hypercubic cell onto pseudospace formed by all other four basic vectors except the two forming the rhombus. The existence domain of the above-mentioned sites on the long face diagonal of rhombus is also a $(RD)_1$, but it is shifted with its center by a distance of $\pm\tau^{-2}(110000)_1$. There are 15 inequivalent 2D faces in a 6D unit cell, and each face has four vertices; hence, there are 60 differently oriented $(RD)_1$ in pseudospace. They overlap with one another and fill the unit tricontahedron, respectively.²²

However, in the case of a standard 3DPT, if two interior vertices of a RD in physical space, denoted as $(RD)_1$, are taken into consideration simultaneously, the existence domain of the face diagonal sites will be enlarged. Two rhombic pyramids which come from the additional interior vertex should be added to each $(RD)_1$ domain. The bases of pyramids coincide with two parallel rhombuses

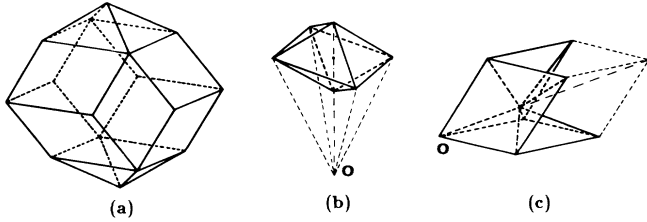


FIG. 4. (a) Two pyramid domains come from the additional interior vertex of the $(RD)_\perp$ are added to the $(RD)_\perp$ existence domain for the face diagonal when two vertices are taken into consideration. (b) The bipyramid existence domain for both occupied or unoccupied face diagonal positions in the interior rhombuses which are shared by two PR. It consists of two pyramids with a common rhombic base. (c) The solid and bold dashed lines show $1/20$ of the existence domain of (Al,Si) -III atoms, which is a triplet consisting of three pyramid domains with a common vertex at the origin. The bases of pyramids are three rhombuses of a $(PR)_\perp$ linking the origin. The thin dashed lines show the $(PR)_\perp$ that one vertex on the long body diagonal is the origin in pseudospace.

forming a $(RD)_\perp$ domain. The distance between the two rhombuses is $\tau^{-1}A$ [Fig. 4(a)]. Hence all the existence domains for face diagonal sites are limited by a unit tricontahedron with 30 rhombic pyramids on its surfaces (described as a horned unit tricontahedron).

It is known from the atomic decoration of α -(Al-Mn-Si) that in a $(RD)_\parallel$ there are four exterior rhombuses of which the two sites on the long face diagonal are all occupied. For other eight exterior rhombuses and two interior rhombuses along the long body diagonal of the $(RD)_\parallel$ only one site is occupied, and the other interior rhombuses are empty [Figs. 1(b) and 1(c)]. Therefore, in order to obtain the existence domain for each inequivalent (Al,Si) -II atom, it is necessary to exclude the existence domains for all the unoccupied face diagonal sites from a $(RD)_\perp$ inside a horned unit tricontahedron. Since the existence domain for all the (Al,Si) -II atoms inside the $(RD)_\parallel$ must have the same shape and size but different position from as that of interior vertices of the $(RD)_\parallel$, it is easily obtained that the existence domains for all the empty interior face diagonal sites are ten pyramids. The bases of pyramids are ten exterior rhombuses of the $(RD)_\perp$ domain and all pyramids point toward its center. Among the ten exterior rhombuses, every four share an exterior vertex on the long body diagonal of the $(RD)_\perp$, and other two are parallel to each other, their distance being $\tau^{-2}A$.

Two remaining exterior rhombuses of the $(RD)_\perp$ domain coincide with the bases of two bipyramids [Fig. 4(b)]. They are the existence domains for the face diagonal sites on the two interior rhombuses of a $(RD)_\parallel$ occupied by (Al,Si) -II atoms. The distance between the bases of two bipyramids is $\tau^{-1}A$. The bipyramids farther distant from the origin of pseudospace correspond to the occupied sites on the long diagonal of rhombuses inside the $(RD)_\parallel$, while the one nearer to the origin corresponds to the unoccupied sites.

As for the unoccupied face diagonal sites on the exterior rhombuses of the $(RD)_\parallel$, the existence domain is the

same as that for the 12-fold vertex in shape and size, but their centers are placed at the positions $\pm\tau^{-2}(\overline{110}000)_\perp$.

Therefore the projection window of each (Al,Si) -II atom is the residual part of the $(RD)_\perp$ existence domain for the face diagonal site after removing the existence domains for all the unoccupied face diagonal sites. It has a very complicated shape, but most of it is distributed around the position $\tau^{-1}(\overline{110}000)_\perp$.

The unit tricontahedron consists of ten PR and ten OR, and the volume ratio of a $(RD)_\perp$ domain to it is 0.2. It can be calculated that the volume ratio of the projection window for each (Al,Si) -II atom is 0.0863. The total ratio is 30×0.0863 or 2.5890.

4. (Al,Si) -III atoms

Obviously, if all the body-center sites inside the standard $(\tau/1)$ projection strip are projected onto pseudospace, their existence domain is also a unit tricontahedron. However, in the atomic decoration of the idealized α -(Al-Mn-Si), only sites on the long body diagonal of a PR inside a $(RD)_\parallel$ are occupied, and each site divides the diagonal in the ratio $\tau^{-1}:\tau^{-2}$. By a similar consideration, it can be obtained that the existence domain of each (Al,Si) -III atom inside a $(RD)_\parallel$ is a rhombic pyramid and one of its base vertices linking the acute angle coincides with the origin in pseudospace. For all 30 differently oriented $(RD)_\parallel$, there are 60 rhombic pyramids around the origin. They form one by one a solid region arranging inside the unit tricontahedron. If 20 prolate rhombohedra are arranged with a common vertex at the origin of pseudospace, the projection window of (Al,Si) -III atoms can be treated as 20 triplets, each of which consists of 3 rhombic pyramids with their common tip located on the long body diagonal of the $(PR)_\perp$ and dividing the diagonal in the ratio $\tau^{-1}:\tau^{-2}$, as shown in Fig. 4(c). The volume ratio is $2\tau^{-3}$.

B. Approximate projection windows

Since the projection windows for i -(Al-Mn-Si) are polyhedra with a very complex shape, it is difficult to calculate the Fourier transform of projection window functions. As an approximation, the projection windows are assumed to be equal-volume solid spheres with different size or spherical shells with different exterior and interior radii; namely, the volume of the sphere or spherical shell is equal to that of the corresponding idealized projection window.

The projection window of Mn atoms can be treated as a spherical shell. Its internal radius equals to the radius of the equal-volume sphere corresponding to the existence domain of MI's centers,

$$R_{11} = 0.1926 A, \quad (2a)$$

and its external radius equals the internal radius of the equal-volume spherical shell corresponding to the existence domain of the internal vertices of the $(RD)_\parallel$,

$$R_{12} = 0.4757 A. \quad (2b)$$

The projection window of (Al,Si) -I atoms located at the

edge center $\pm(\frac{1}{2}00\ 000)_{\parallel}$ is approximated as two spheres placed at the position $\pm(\frac{1}{2}00\ 000)_{\perp}$. The radius of spheres is given by

$$R_2 = R_{11} = 0.1926 A . \quad (3)$$

The projection window of one kind of (Al,Si)-II atoms has a very complicated shape, but most of it distributes around the position $\tau^{-1}(110\ 000)_{\perp}$, which corresponds to the atomic position $\tau^{-1}(110\ 000)_{\parallel}$ on the long face diagonal or rhombuses linking the MI centers in physical

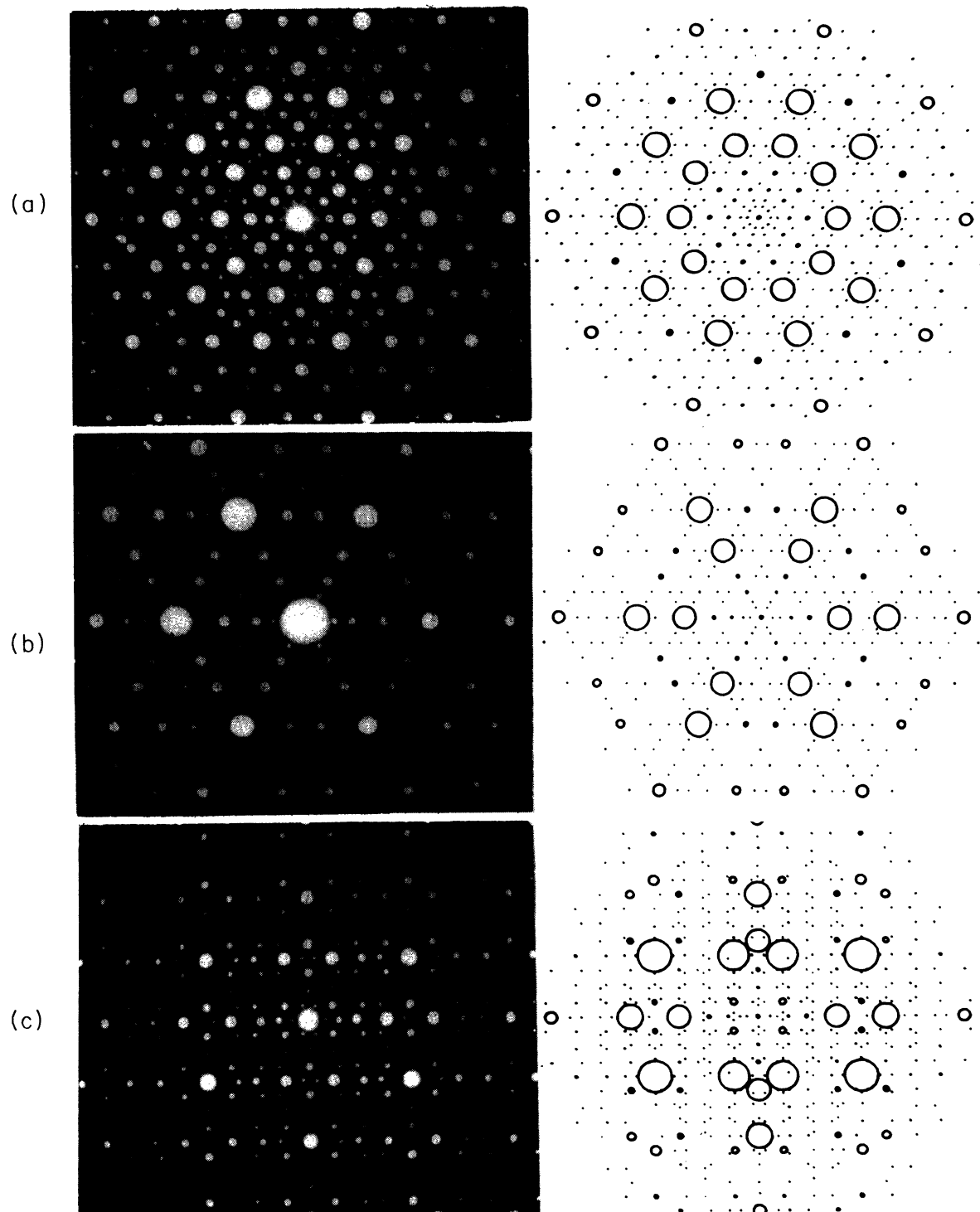


FIG. 5. Observed (left) and calculated (right) electron-diffraction patterns of obtained *i*-(Al-Mn-Si) along the (a) fivefold axis, (b) threefold axis, and (c) twofold axis. The areas of the circles are proportional to the intensity of the diffraction spots.

space. Therefore the projection window can be also treated as an equal-volume sphere placed at the position $\tau^{-1}(110\ 000)_\perp$. Its radius is given by

$$R_3 = 0.2300 A . \quad (4)$$

The projection window of (Al,Si)-III atoms can be treated as a sphere with radius

$$R_4 = 0.4052 A . \quad (5)$$

C. Comparison between calculated and experimental electron diffraction patterns

The calculation of the structure factor is performed with the formula

$$F(H_{\parallel}, H_{\perp}) = \exp[-BH_{\parallel}^2/4 - B'H_{\perp}^2/4] \times \sum_{j=1}^n P_j f_j(H_{\parallel}) S_j(H_{\perp}) \exp(2\pi i H R_j) . \quad (6)$$

Here R_j is the atomic coordinate of 6D hypercubic-crystal-lattice atoms, H is the 6D reciprocal vector, H_{\parallel} and H_{\perp} are the components of H in physical and pseudospaces, respectively, $f_j(H_{\parallel})$ is the atomic scattering factor for electrons, $S_j(H_{\perp})$ represents the Fourier transform of the projection windows of 6D hypercubic-crystal-lattice atoms, and P_j is the atomic occupation. B is the isotropic overall temperature factor, and B' is an additional factor due to the phason effect.

Figure 5 shows the observed electron-diffraction patterns of *i*-(Al-Mn) in the left-hand side. They are taken along the (a) fivefold, (b) threefold, and (c) twofold axes, respectively. The electron-diffraction patterns of *i*-(Al-Mn-Si) calculated with the approximate projection windows are shown in the right-hand side. The atomic scattering factors for electrons are calculated by using the analytical formula with nine parameters.²³ The temperature factor $B = 4 \text{ \AA}^2$ and the additional factor $B' = 65 \text{ \AA}^2$ were used. The atomic occupation $P_j = 1$. It can be seen that the calculated electron-diffraction patterns are coincident in the main with the experimental patterns of *i*-(Al-Mn).

D. Chemical composition and density

According to such an obtained structural model of *i*-(Al-Mn-Si), the chemical composition and density are (Al,Si)_{5.15}Mn and 3.64 g cm^{-3} , respectively, which are close to those of idealized α -(Al-Mn-Si).

VI. DISCUSSION AND CONCLUSIONS

A 6D hypercubic crystal-structure model has been constructed by using a previously developed method based

on the projection description. This method is first used on *i*-(Al-Mn-Si). The 6D atomic coordinates are derived from the 3D atomic coordinates in α -(Al-Mn-Si). The multisolution problem in the 6D crystal-structure construction is solved by assigning a special solution on the basis of the rhombic tiling for bcc structure. This 6D crystal-structure model is similar to but different from those previously reported. There are altogether 38 atoms in the 6D unit cell, and the number of inequivalent atoms is 4. The idealized projection windows for different kinds of inequivalent atom in the 6D hypercubic crystal-structure model are polyhedra determined on the basis of the similarity between the local atomic arrangements of *i*-(Al-Mn-Si) and those of α -(Al-Mn-Si) and between the local environments of 3DPT and those of the rhombic tiling. Projections of the 6D hypercubic crystal onto physical space with the determined ($\tau/1$) and ($1/1$) projection strips give the idealized *i*-(Al-Mn-Si) and α -(Al-Mn-Si), respectively.

The structure of *i*-(Al-Mn-Si) obtained by using the idealized projection windows consists of MI's and linking atoms with reasonable atomic bonds and local clusters, and the positions of MI's and distribution of linking atoms with different local atomic arrangements in it are also reasonable. In principle, the projection method is identical to the cut method. However, for the latter the high-dimensional atoms extend along pseudospace to form the so-called existence domains. It is evident that the existence domains for different atoms should not overlap. In the case of the projection method, the projection of a high-dimensional atom onto the physical space gives the real atom, while that in pseudospace gives a geometric point. The shape of a projection window for the projection method is equivalent to the shape of existence domain for the cut method. But the projection windows determined in the present paper correspond to the existence domains for the cut method, which are allowed to overlap. This is one more difference of the present model from other models.

The present method of constructing the 6D crystal-structure model is expected to be generally applicable to all icosahedral quasicrystals which coexist with a bcc or an almost bcc crystalline approximant. It is possible to develop similar methods of constructing 6D crystal-structure models for icosahedral quasicrystals with crystalline approximants other than the bcc crystal lattice and of constructing high-dimensional crystal-structure models for different kinds of quasicrystal on the basis of the same principles.

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¹L. A. Bendersky and M. J. Kaufman, *Philos. Mag.* B 53, L75 (1986).

²V. Elser and C. L. Henley, *Phys. Rev. Lett.* 55, 2883 (1985).

³J. W. Cahn and D. Gratias, *J. Phys. (Paris)* 47, C3-415 (1986).

⁴P. Guyot and M. Audier, *Philos. Mag.* B 52, L15 (1985).

⁵M. Audier and P. Guyot, *Philos. Mag.* B 53, L43 (1986).

⁶Q. B. Yang, *Philos. Mag.* B 58, 47 (1988); *Lett.* 41, 145 (1985).

⁷A. Yamamoto and K. Hiraga, *Phys. Rev. B* 37, 6207 (1988).

⁸J. W. Cahn, D. Gratias, and B. Mozer, *Phys. Rev. B* 38, 1638

- (1988).
- ⁹D. Gratias, J. W. Cahn, and B. Mozer, *Phys. Rev. B* **38**, 1643 (1988).
- ¹⁰J. W. Cahn, D. Gratias, and B. Mozer, *J. Phys. (Paris)* **49**, 1225 (1988).
- ¹¹A. Yamamoto, in *Quasicrystals*, Springer Series in Solid-State Science, Vol. 93, edited by T. Fujiwara and T. Ogawa (Springer, New York, 1990), p. 57.
- ¹²M. Duneau and C. Oguey, *J. Phys. (Paris)* **50**, 135 (1989).
- ¹³Y. Ma, E. A. Stern, and C. E. Bouldin, *Phys. Rev. Lett.* **57**, 1611 (1986).
- ¹⁴E. A. Stern and Y. Ma, *Philos. Mag. Lett.* **56**, 103 (1987).
- ¹⁵A. L. Mackay, *Acta Crystallogr.* **15**, 916 (1962).
- ¹⁶G. Z. Pan, Y. F. Cheng, and F. H. Li, *Phys. Rev. B* **41**, 3401 (1990).
- ¹⁷M. Cooper and K. Robinson, *Acta Crystallogr.* **20**, 614 (1966).
- ¹⁸T. Janssen, *Acta Crystallogr. A* **42**, 261 (1986).
- ¹⁹R. Penrose, *Bull. Inst. Math. Appl.* **10**, 266 (1974).
- ²⁰Y. F. Cheng, G. Z. Pan, and F. H. Li (unpublished).
- ²¹C. L. Henley, *Phys. Rev. B* **34**, 797 (1986).
- ²²A. Katz, in *Introduction to the Mathematics of Quasicrystals*, edited by Marko V. Jarić, *Aperiodicity and Order*, Vol. 2 (Academic, San Diego, 1989), Chap. 4, pp. 147–182.
- ²³J. S. Jiang and F. H. Li, *Acta Phys. Sin.* **33**, 845 (1984).

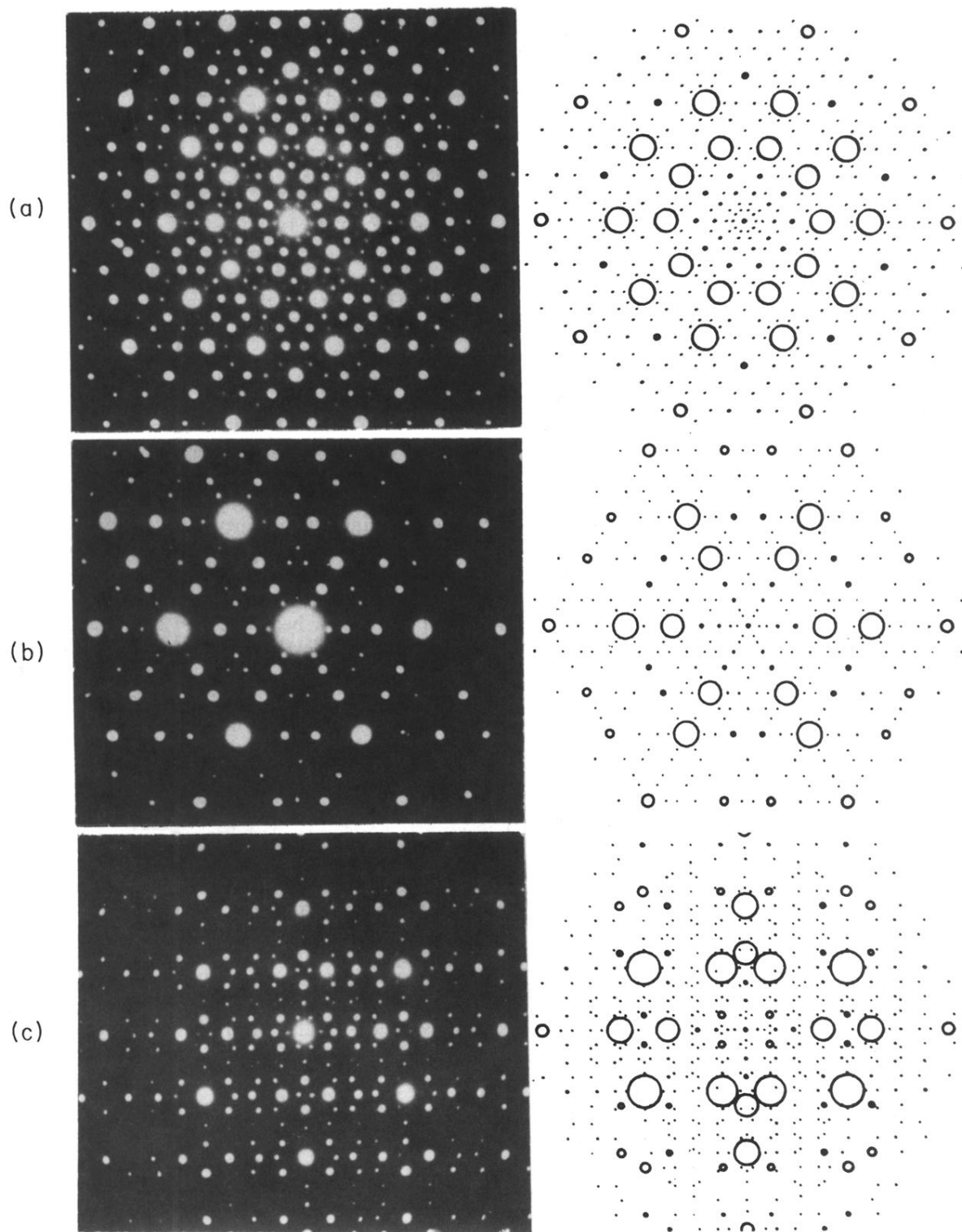


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