Ideal structure of icosahedral Al-Cu-Li quasicrystals

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A structure model for the icosahedral Al-Cu-Li quasicrystal has been derived. This is described in six-dimensional space as a six-dimensional crystal, having four kinds of occupation domains with complicated polyhedral shape. A general structure-factor formula is derived for such polyhedral domains, and a simple description of the structure using the site symmetry is proposed. The model gives R factors of 0.076 and 0.085 for recent x-ray and neutron-single-crystal-diffraction data [Boissieu, Janot, Dubois, Audier, and Dubost, J. Phys. **3**, 1 (1991)]. The structure consists of a large number of icosahedral clusters and linking atoms joining them. It leads to an ideal cubic R-Al-Cu-Li structure and a large number of other cubic crystals when appropriate phason strains are taken into account. Two structures, the ideal R-Al-Cu-Li structure and a fictitious structure with a period $(1+\sqrt{5})/2$ times longer, are shown.

I. INTRODUCTION

Since the discovery of icosahedral Al-Mn,[1] many theoretical and experimental studies have been made to clarify quasicrystal structures[2–20] and determined the approximate structures of icosahedral quasicrystals. In particular, realistic models that can explain the diffraction intensities of icosahedral Al-Mn and Al-Cu-Li have been given. The model for icosahedral Al-Mn (i-Al-Mn) proposed by Yamamoto and Hiraga[16] (YH model) consists of many icosahedral clusters (Mackay icosahedra) situated at the 12-fold vertices in the three-dimensional Penrose pattern (3DPP) and linking atoms joining them. In the model of icosahedral Al-Cu-Li (i-Al-Cu-Li) by Elswijk *et al.*[17,18] (EHSB model), the vertex and edge-center positions in the 3DPP are mainly occupied by Al and Cu, and two positions in the body diagonal of the acute rhombohedron in the 3DPP are mainly occupied by Li. These models explain well the diffraction intensity. They are therefore important as starting models for a further study, but not ideal as models because they include some atomic disorder.

In the YH model, the linking Mn and Al atoms are disordered and are placed with the occupation probability of $\frac{1}{2}$, while in the EHSB model, all the sites (vertex, edge-center, and body-diagonal positions) are partially occupied by Al, Cu, and Li. It is uncertain whether such disorder is present in real quasicrystals. The YH model, in addition, includes a small number of short interatomic distances that are crystallographically unreasonable. In order to improve these points, Duneau and Oguey[19] gave a slightly different model for i-Al-Mn (DO model) but the model does not lead to the structure of the cubic approximant, α-Al-Mn-Si, under an appropriate cubic phason strain.[21] The EHSB model includes lots of atom clusters as in its cubic approximant, R-Al-Cu-Li, but in contrast to the approximant, many clusters do not have icosahedral symmetry. It seems quite natural from the crystal-approximant structure that i-Al-Cu-Li or i-Al-Mn also consists of icosahedral clusters and the linking atoms joining them. In this paper we consider a quasicrystal model that has a local atom arrangement similar to that of R-Al-Cu-Li and gives an ideal R-Al-Cu-Li structure under the appropriate phason strain.

There are three approaches to model quasicrystal structures. The first one is the section (projection) method in which the quasicrystal structure is given as the three-dimensional section of a higher-dimensional crystal.[2–9] The second is the inflation method in which the structure is constructed by the matching rules.[10–12] The last one is the dual (generalized dual) method which uses dual transformation to obtain a quasiperiodic structure from a periodic or quasiperiodic grid in three-dimensional space.[13–15] Among them the most convenient method for the structure analysis based on diffraction experiments is the section method, which is employed in this paper.

In the section method, the icosahedral structure is described as a six-dimensional crystal which has atoms with occupation (acceptance) domains extended over the internal (perpendicular or complementary) space. The structure in the external (parallel or real) space is given by the three-dimensional intersection of the six-dimensional crystal. This gives a simple method for calculating the structure factor. Therefore, if we can construct a model of the six-dimensional crystal, its structure factor can be compared with experiment. The model can be constructed by the theoretical consideration of the crystal approximant and 3DPP.

Another approach has been taken by two groups to analyze quasicrystal structure. In this method, the phase of the observed structure factor is determined by the structure factor of the cubic crystal approximant R-Al-Cu-Li or by the contrast-variation method in neutron scattering.[22,23] This provides the electron density of a six-dimensional crystal by direct Fourier transformation of the structure factor, from which the approximate shape of occupation domains can be deduced. This approach, however, still needs a model for the quasicrystal. The electron density in the internal space is obscure because many weak diffraction intensities are unobservable, so that there exists an ambiguity in determining the shape of

the occupation domain.

We employ the former method in this paper and describe an improved model for *i*-Al-Cu-Li which was proposed previously[21] in more detail. The model includes neither nonphysical interatomic distances nor partially occupied sites with occupation probability less than one, except for the intrinsic disorder in Al and Cu. It contains many icosahedral clusters and gives reasonable values for the chemical composition and density.

In addition to the determination of real quasicrystal structures, some theoretical works on quasicrystals, for example electron-energy-band calculations or simulations of the structure image in electron microscopy, need periodic structures. For such works, it is useful to derive a series of crystal structures with different unit-cell dimension but with cubic symmetry and a local atom arrangement similar to that of the quasicrystal. Once we obtain a quasicrystal model described in six-dimensional space, we can derive such a series of crystal structures by considering an appropriate phason strain and taking a three-dimensional section as shown below. The procedure employed[24,25] is equivalent to that shown by Elser[5] for a one-dimensional analogue of the quasicrystal and similar to the method by Kramer[26] for the 3DPP, but we use the section method here.[16] We derive two cubic structures from the quasicrystal model, one of which is an idealized structure for a real cubic crystal (*R*-Al-Cu-Li) and the other is a hypothetical one with a simple-cubic lattice and lattice dimension τ times larger than that of the former. [τ is the golden ratio $(1+\sqrt{5})/2$.] The derived structures give correct space-group symmetry: the body-centered $Im3$ is in agreement with the real structure for the former while the latter must have $Pm3$ as shown by Kramer.[26]

The purposes of the present paper are to construct a model without unnecessary disorder and unacceptable short interatomic distances for the *i*-Al-Cu-Li quasicrystal, and to derive from the model related cubic crystal structures found in several theoretical works. Furthermore it is shown by structure-factor calculations that the model is a realistic model for *i*-Al-Cu-Li and can explain the observed x-ray- and neutron-diffraction intensities obtained from single-crystal diffraction experiments.[23] A general structure-factor formula which is applicable to any icosahedral quasicrystal with polyhedral occupation domains is given. This includes the symmetry operations explicitly, so that we can calculate the structure factor by specifying only independent parts of the occupation domains. The description of the occupation domain is simplified by the use of site symmetry. This is demonstrated.

The arrangement of the paper is as follows. In Sec. II, we describe the occupation domains for a simple decoration model and an ideal model. The structure-factor formula for a general icosahedral structure is given in Sec. III. The refinement of the ideal model is made by using recent x-ray- and neutron-diffraction data in Sec. IV. Finally, in Sec. V, we derive an ideal *R*-Al-Cu-Li structure and a fictitious cubic structure with a τ-times larger unit-cell dimension from the quasicrystal model under the phason strain.

II. DERIVATION OF OCCUPATION DOMAINS

In the section method,[8,9,16] the quasicrystal structure is described by a crystal in superspace which has several occupation domains. For an icosahedral quasicrystal, such a crystal structure is conveniently described by the icosahedral coordinate system in six-dimensional space. The six-dimensional space is divided into two three-dimensional subspaces. One of them is called the external (real or parallel) space and the other, the internal (complementary or perpendicular) space. Each atom position is given as an intersection of the occupation domain spreading over the internal space on the external space.

The unit vectors of the icosahedral lattice are given by $\mathbf{a}_1=\alpha(1,\tau,0,\tau,-1,0)_0$, $\mathbf{a}_2=\alpha(\tau,0,1,-1,0,\tau)_0$, $\mathbf{a}_3=\alpha(\tau,0,-1,-1,0,-\tau)_0$, $\mathbf{a}_4=\alpha(0,1,-\tau,0,\tau,1)_0$, $\mathbf{a}_5=\alpha(-1,\tau,0,-\tau,-1,0)_0$, $\mathbf{a}_6=\alpha(0,1,\tau,0,\tau,-1)_0$, where $\alpha=a/\sqrt{(2+\tau)}$ with $a=5.06$ Å (a being the lattice constant of the icosahedral lattice). The first three components are the orthogonal coordinates of the external space (with respect to the unit vectors $\mathbf{a}_{01}$, $\mathbf{a}_{02}$, and $\mathbf{a}_{03}$) and the latter three are those of the internal space (referred to $\mathbf{a}_{04}$, $\mathbf{a}_{05}$, and $\mathbf{a}_{06}$). The coordinates with respect to $\mathbf{a}_{0j}$ are distinguished by the subscript 0 from those of $\mathbf{a}_j$. These unit vectors are equivalent to $\mathbf{a}_1=a(0,0,1,0,0,1)_0$, $\mathbf{a}_j=a(c_j s, s_j s, c, -c_{2j} s, -s_{2j} s, -c)_0$ [$j=2,3,\ldots,6$, $c_j=\cos(2\pi j/5)$, $s_j=\sin(2\pi j/5)$, $c=1/\sqrt{5}$, $s=2/\sqrt{5}$] used in a previous paper[16] but the unit vectors of the external and internal spaces are selected so as to be directed at the twofold axes in the present case for the convenience of the cubic phason strain mentioned later. (It should be noted that the vectors $\mathbf{a}_{0j}$ are different from those assumed by Cahn *et al.*[27])

The coordinates define the transformation matrix M which relates the unit vectors of the six-dimensional lattice with the unit vectors of the external and internal spaces: $\mathbf{a}_i=\sum_j M_{ij}\mathbf{a}_{0j}$. As is well known, the projection of the unit cell or the Wigner-Seitz cell onto the internal space is the rhombic triacontahedron with the edge length of a [Fig. 1(a)].[4] The 3DPP is a basic pattern for

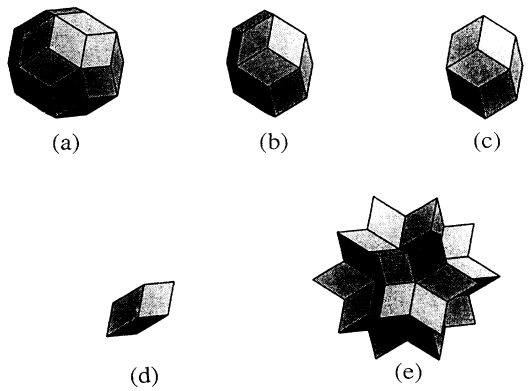

FIG. 1. Occupation domains appearing in the three-dimensional Penrose pattern and its simple decoration. (a) Rhombic triacontahedron, (b) rhombic icosahedron, (c) rhombic dodecahedron, (d) acute rhombohedron, and (e) D_{1E} dodecahedron with the edge length equal to the lattice constant a.

icosahedral quasicrystals and is given by the intersection of the six-dimensional crystal in which the occupation domain shown in Fig. 1(a) is placed at each lattice point. It is well known that the 3DPP consists of two kinds of rhombohedra called the acute and obtuse ones, each of which has the same edge length equal to the lattice constant a.[4,13] A realistic quasicrystal model is obtained from it by adding additional atom positions.

(a) Simple decoration. A simple decoration model for *i*-Al-Cu-Li includes additional occupation domains which are common parts of two or more rhombic tricontahedra (RT) placed at different positions. The edge-center position is obtained from the rhombic icosahedron placed at $(1,0,0,0,0,0)/2$, which is the *common part* of two RT placed at the origin and $(1,0,0,0,0,0)$ when the two domains are projected onto the internal space[28,29] [Fig. 1(b)]. Similarly, the body-center position of the acute rhombohedron in the external space can be derived from the common part of four RT placed at the origin, $(1,0,0,0,0,0)$, $(0,1,0,0,0,0)$, and $(0,0,1,0,0,0)$. This is the acute rhombohedron (spreading in the internal space) placed at $(1,1,1,0,0,0)/2$ [Fig. 1(d)]. [The rhombic dodecahedron in Fig. 1(c) is related to the face-center position but is not relevant for awhile.[28]] In a simple model for *i*-Al-Cu-Li, Al and Cu occupy the vertex and edge-center positions at random.[30]

Li atoms occupy two body-diagonal positions of the acute rhombohedron,[17] which divide the body diagonal into the ratio $\tau^{-2}:\tau^{-3}:\tau^{-2}$. The occupation domain for the Li atoms is given by the acute rhombohedron at $(1,1,1,0,0,0)/2\pm(0,0,0,1,\bar{1},1)^e/2$, where the superscript e means the external-space components of a six-dimensional vector. (The internal-space component is expressed by the superscript i.) Since $(0,0,0,1,\bar{1},1)^e/2$ is equivalent to $(0,0,0,1,\bar{1},1)/2-(0,0,0,1,\bar{1},1)^i/2$, the Li site is given by the acute rhombohedron at $(1,1,1,1,1,1)/2\pm(0,0,0,1,\bar{1},1)^i/2$ and its equivalent positions under the icosahedral symmetry. The symmetry operators of the icosahedral group generate 20 acute rhombohedra around the body center $(1,1,1,1,1,1)/2$ forming the dodecahedron shown in Fig. 1(e). We will call this the D_{1E} dodecahedron. Thus, the simple model of *i*-Al-Cu-Li is given by three domains shown in Figs. 1(a), 1(b), and 1(e).

It should be noted that the vertex and edge-center positions come from the occupation domains at the origin and edge center of the six-dimensional icosahedral lattice but the two body-diagonal positions are obtained from that placed at the body center. In general, it can be shown that the position $\tau^{-1}a$ apart from a vertex of the 3DPP along a fivefold axis is obtained from an occupation domain at the body center or around it in the internal space. We call such positions edge-off-center positions. The two body-diagonal positions are such examples.

(b) Ideal structure. The model mentioned above can explain the diffraction intensity very well provided that each position is statistically occupied by Li, Al, and Cu.[17,18] Such a statistical occupation of one position with Li, Al, and Cu, however, seems to be unnatural and suggests that the real structure has more complicated occupation domains which are occupied by either Li or Al and Cu. The statistical occupation of one site by Al and Cu may be intrinsic in this case because such an occupation is seen in the crystal approximant *R*-Al-Cu-Li with the cubic space group $Im3$.[31–33]

R-Al-Cu-Li can be considered to consist of two units.[34] One of them is the rhombic dodecahedron [Fig. 2(a)] and the other is the acute rhombohedron [Fig. 2(c)]. In another view, the structure includes two icosahedral clusters at the origin and body center, each of which consists of 24 Al or Cu and 20 Li. We call these points the 12-fold vertices because they correspond to the 12-fold vertex in the 3DPP. Since the cluster center is vacant, the 12-fold vertex itself is not occupied by an atom.[33] The characteristic feature of the crystal is that the 12-fold vertices are connected either with the acute rhombohedron or with the rhombic dodecahedron mentioned above as in the 3DPP.

As an ideal quasicrystal structure, we consider the structure that has a local atom arrangement as close as possible to that of *R*-Al-Cu-Li. We place the same icosahedral atom clusters at the 12-fold vertices and connect the 12-fold vertices with the two units with the same decorations as those of the crystal approximant (Fig. 2). In order to realize such a local atom arrangement in the quasicrystal, we have to consider three points. First, the 12-fold vertices are removed because the cluster center is not occupied; second, vertex positions with unacceptable nearest-neighbor distances have to be removed; and finally, some edge-center positions are shifted to the edge-off-center positions.

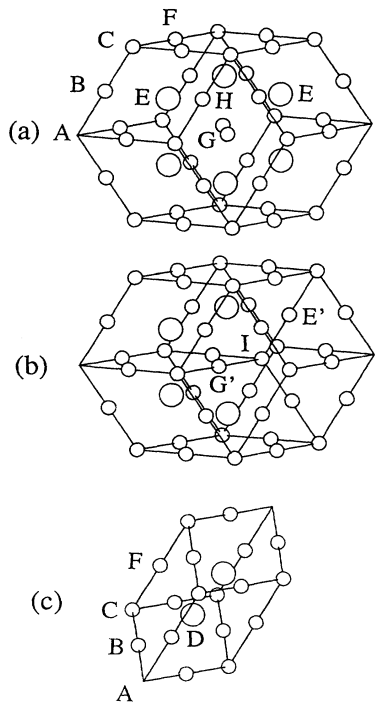

FIG. 2. Decoration of the two structural units in *R*-Al-Cu-Li and the simple decoration model. The rhombic dodecahedra in (a) the former and (b) the latter. The acute rhombohedron (c) is common to both cases.

It is known that the 12-fold vertices are obtained from the small rhombic triacontahedron (SRT) with edge length of $\tau^{-2}a$.[16,35] If we place the icosahedral clusters at all of them, a small number of clusters interpenetrate each other. Such a situation is not seen in the crystal approximant. The appearance of the clusters in such a short distance can be avoided by placing the clusters at the 12-fold vertices that are derived from the occupation domain shown in Fig. 3(a). This is obtained from the SRT after dropping the cap along the fivefold axis. We call this a small truncated rhombic triacontahedron (STRT). To remove the relevant 12-fold vertices, therefore, the STRT has to be removed from the central part of the occupation domain shown in Fig. 1(a).

With respect to the second point, we have to remove small domains from the RT as shown below. The icosahedral cluster consists of 12 edge-center Al or Cu atoms at $(1,0,0,0,0,0)^e/2$ (and its equivalent positions), 12 Al or Cu at $(1,0,0,0,0,0)^e$, and 20 Li at $(0,0,0,1,\bar{1},1)^e$. When the cluster is placed at every 12-fold site, the vertex in the rhombic dodecahedron (RD) connecting two 12-fold vertices [I in Fig. 2(b)] should be removed because it is unacceptably near an edge-off-center position of the RD [E and G in Fig. 2(a)]. The vertex to be removed is $(0,1,0,1,0,0)^e$ apart from the 12-fold site, which is obtained from the STRT at $(0,1,0,1,0,0)^i$. Therefore, the common part of the RT at the origin and the STRT mentioned above (and equivalent to it) has to be removed. The resulting shape is shown in Fig. 3(b). Here and hereafter the SRT is used instead of the STRT for convenience.

In the inside of the RD, the edge-center positions in the simple decoration [E' and G' in Fig. 2(b)] have to be shifted into the edge-off-center positions (E and G). The edge-center E' site is located at $(\bar{1},2,0,0,0,0)^e/2$ (from the 12-fold vertex) which is equal to $(1,0,0,0,0,0)/2+(1,\bar{2},0,0,0,0)^i/2$ modulo the lattice vector. Therefore, the STRT placed here has a common part to the rhombic icosahedron (RI) [Fig. 1(b)] at the edge-center $(1,0,0,0,0,0)/2$. Similarly, the edge-center G' site at $(1,2,0,0,0,0)^e/2$ (measured from the 12-fold vertex) is equivalent to $(1,0,0,0,0,0)/2-(1,2,0,0,0,0)^i/2$ and the STRT has also a common part to the RI at $(1,0,0,0,0,0)/2$. The rhombic icosahedron after removing these common parts is shown in Fig. 3(c).

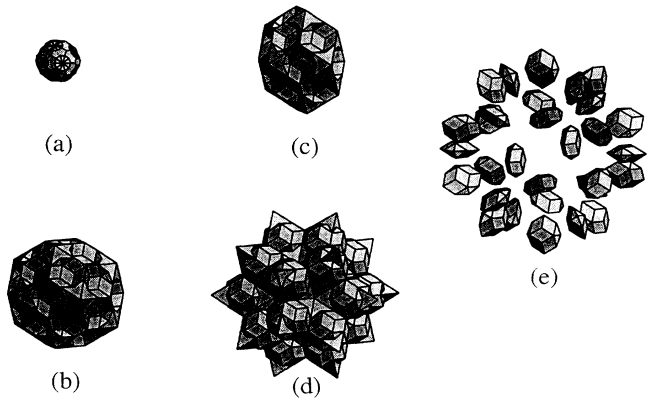

FIG. 3. Occupation domains of the ideal structure for (a) vacant 12-fold, (b) vertex Al,Cu, (c) edge center Al,Cu, (d) edge-off-center Li, and (e) edge-off-center Al,Cu sites. The domain with the shape of (a) is subtracted from the central part of (b) to remove unoccupied 12-fold vertices.

Finally, several edge-off-center positions have to be added. The occupation domains for the edge-off-center E sites and equivalent to them are given by the STRT at $-(\bar{1},\bar{1},1,1,1,1)^e/2$ because $(\bar{1},2,0,0,0,0)^e/2$ is shifted there and this is equivalent to $(1,1,1,1,1,1)/2+(\bar{1},\bar{1},1,1,1,1)^i/2$. [Note that $\tau^{-1}(1,0,0,0,0,0)^e$ is equal to $(\bar{1},1,1,1,1,1)^e/2$.] The position $(\bar{1},\bar{1},1,1,1,1)^i/2$ is on the body diagonal of an acute rhombohedron of the D_{1E} dodecahedron [Fig. 1(e)] and it divides the body diagonal into the ratio $\tau^{-1}:\tau^{-2}$. Therefore, the two body-diagonal positions included in the simple decoration and additional edge-off-center E sites are obtained from the union of the D_{1E} dodecahedron and the 20 STRT's [Fig. 3(d)]. Similar consideration for the edge-off-center G sites leads to the occupation domain shown in Fig. 3(e). Thirty "capped" rhombic dodecahedra with the edge length of $\tau^{-2}a$ are located around $(1,1,1,1,1,1)/2$. These are on the twofold axis and share two edges with the occupation domain in Fig. 3(d).

Since the edge-center and its nearest edge-off-center positions are too short to be occupied at the same time, their occupation domains are inhibited from overlapping when they are projected onto the internal space. If the location in the external space is neglected, the occupation domain for the edge-center positions [Fig. 3(c)] is located in the internal space on the D_{1E} dodecahedron [Fig. 3(d)] and contact its five concave faces around the fivefold axis with five convex faces of the latter around the same axis. Then the concave parts in the former agree with the convex parts of the latter. On the other hand, the occupation domains of the edge-off-center G sites [Fig. 3(e)] come to the outer five concave faces of the rhombic icosahedron [Fig. 3(c)]. Thus, the overlap of the occupation domains are avoided.

In R-Al-Cu-Li, the edge-off-center E site [Fig. 2(a)] is occupied by Li while the G site is occupied by Al.[33] In the simple decoration model mentioned previously, the edge-center position is partially occupied by Li with small occupation probability.[17] This suggests that the edge-off-center E site is occupied by Li as in R-Al-Cu-Li. The small occupation probability of Li in the vertex position of the simple decoration model[17] seems to be related with the fact that a vertex in the rhombic dodecahedron connecting the 12-fold vertices [I in Fig. 2(b)] is unoccupied since the Li atom is hard to observe by x-ray diffraction.

In summary, Al and Cu statistically occupy the occupation domains shown in Figs. 3(b), 3(c), and 3(e) while Li occupies that in Fig. 3(d). In particular, the occupation domain of Fig. 3(e) is expected to be completely occupied by Al. The structure-factor calculation will show that such an arrangement of chemical species is realized in the i-Al-Cu-Li quasicrystal.

III. STRUCTURE FACTOR

As shown in the previous section, the occupation domain is generally a complicated polyhedron with con-

cave parts. The structure factor of the quasicrystal with the diffraction vector $\mathbf{q}$ is given by the summation of the Fourier integrals of such occupation domains:

$$F(\mathbf{q})=\sum_{\{R|\tau\}}\sum_{\mu}a^{\mu}f^{\mu}(q^{e})p^{\mu}\exp(-B^{\mu}q^{e2}/4)\times\exp(2\pi i\mathbf{q}\cdot[R\mathbf{r}^{\mu}+\tau])F^{\mu}(R^{-1}\mathbf{q}) , \quad (1)$$

where a^{μ}, $f^{\mu}(q^{e})$, p^{μ}, and B^{μ} are the (inverse of) multiplicity, atomic scattering factor, occupation probability, and isotropic temperature factor of the μth independent atom in the unit cell, and $F^{\mu}(\mathbf{q})$ is the Fourier integral of the occupation domain at the position $\mathbf{r}^{\mu}$. The summation with respect to the symmetry operator $\{R|\tau\}$ runs over the symmetry operators which generate equivalent atoms in the unit cell from independent ones as in the usual structure-factor formula. If we consider the temperature factor B'^{μ} coming from the random phason, the factor $\exp(-B^{\mu}q^{e2}/4)$ is replaced by $\exp(-B^{\mu}q^{e2}/4-B'^{\mu}q^{i2}/4)$ in Eq. (1).

A convex polyhedron can be divided into several tetrahedra, each of which is defined by three vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ directed from the center of the polyhedron to the three corners other than the corner at the center. If a polyhedron has concave parts, the polyhedron is obtained from some convex polyhedron by removing the concave parts. Its Fourier integral is given by the contribution of the convex polyhedron minus that of the concave parts owing to the linearity of the Fourier integral. In Eq. (1), the concave parts are treated as occupation domains with $p=-1$. (Note that the concave part to be removed is a convex polyhedron so that it can be divided into tetrahedra.) Thus, the calculation of the structure factor is reduced to that of the Fourier integral of the tetrahedron, which can be calculated analytically as shown below.

As shown in the Appendix the Fourier integral of the tetrahedron defined by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ is given by

$$F_0(\mathbf{q})=-iV[q_2q_3q_4\exp(iq_1)+q_3q_1q_5\exp(iq_2)+q_1q_2q_6\exp(iq_3)+q_4q_5q_6]/(q_1q_2q_3q_4q_5q_6) , \quad (2)$$

where $q_j=2\pi\mathbf{q}\cdot\mathbf{e}_j$ $(j=1,2,3)$, $q_4=q_2-q_3$, $q_5=q_3-q_1$, $q_6=q_1-q_2$, and $V=\mathbf{e}_1\cdot[\mathbf{e}_2\times\mathbf{e}_3]$ is the volume of the parallelepiped defined by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$. [It should be noted that q_j depends only on the internal space component of $\mathbf{q}$ because $\mathbf{e}_j$ is a vector in the internal space. Consequently, $F_0(\mathbf{q})$ also depends only on the internal space component of $\mathbf{q}$.]

In order to calculate the Fourier integral of a polyhedron, it is convenient to use the site-symmetry operations under which the polyhedron is unchanged. Then the Fourier integral of the polyhedron can be calculated from that of its independent part by using the site-symmetry operations. Provided that the independent part consists of n tetrahedra, the Fourier integral of the polyhedron is expressed as

$$F^{\mu}(\mathbf{q})=\sum_{\{R_s|\tau\}}\sum_{j=1}^{n}F_0^j(R_s^{-1}\mathbf{q}) \quad (3)$$

with the site-symmetry operation $\{R_s|\tau\}$ and the Fourier integral for the jth (independent) tetrahedron, $F_0^j(\mathbf{q})$, which is given by Eq. (2). For example, the Fourier integral of the rhombic triacontahedron [Fig. 1(a)] can be derived from that of one tetrahedron by the site-symmetry operations. Since it is located at the origin and has full icosahedral symmetry, its independent part is the tetrahedron which is defined by three vectors $\mathbf{e}_1=-(\bar{1},1,1,1,1,1)^i/2$ (fivefold corner of the RT), $\mathbf{e}_2=(1,1,1,1,\bar{1},1)^i/2$ (threefold corner), and $\mathbf{e}_3=(1,1,0,0,\bar{1},1)^i/2$ (face center). For the rhombic icosahedron [Fig. 1(b)] at $(1,0,0,0,0,0)/2$, the independent part is two tetrahedra and the D_{1E} dodecahedron [Fig. 1(e)] at $(1,1,1,1,1,1)/2$ can be derived from one tetrahedron. These are defined by vectors shown in Table I. (In the above examples, the site symmetry of the occupation domain center coincides with the symmetry of the occupation domain itself but, in general, the symmetry of the occupation domain may be higher than the site symmetry.)

As stated in the previous section, the quasicrystal structure can be described by specifying the shape of each occupation domain and its location. The use of the site symmetry and the independent tetrahedra provides a convenient method for specifying the shape of the occupation domain. Thus, the decomposition of the occupation domain into independent tetrahedra is efficient not only for the convenience of structure-factor calculations but also for a simple description of the quasicrystal.

IV. REFINEMENT OF THE STRUCTURE

The diffraction intensity of the i-Al-Cu-Li model described in Sec. II can easily be calculated with the use of the structure-factor formula given in the previous section. To specify the shape of polyhedral occupation domains, it is sufficient to give three edge vectors for each independent tetrahedron after dividing the occupation domain into tetrahedra with positive and negative occupation probabilities. The edge vectors for the present model are listed in Table I. Refinable parameters in the present model are the temperature factor B^{μ} and B'^{μ} for each occupation domain and the occupation probability p of Al for the Al,Cu site. (The occupation probability of Cu is given by $1-p$.) We employed the recent intensity data for single-crystal x-ray and neutron diffraction by Boissieu *et al.*[23] The least-squares program based on the structure-factor formula described above has been written and applied to the calculation of diffraction intensities of the Hiraga-Hirabayashi model in i-Al-Mn.[16] This was extended to use x-ray- and neutron-diffraction data simultaneously: It minimizes the sum of the weighted R factors for x-ray and neutron data by the least-squares

TABLE I. The vectors defining independent polyhedra. Each vector $\mathbf{e}_j$ represents the position of the corner measured from the center of an occupation domain at $\mathbf{r}+\mathbf{r}^i$. Consecutive three vectors define a tetrahedron. A negative p in the header means a concave part. The occupation domain is generated from the listed tetrahedra by the site symmetry G_s given in the heading. [$\tau^{-1}=0.61803$, $\tau^{-2}=0.31897$, $\tau^{-3}=0.23607$, $\tau^{-3}/2=0.11803$, $\tau^{-2}/2=0.19099$, $(3-\tau^{-2})/2=1.30902$].

(a) Vectors defining the small truncated rhombic triacontahedron (STRT) [Fig. 3(a)], which has to be removed from the central part of Fig. 3(b).

(STRT) $G_s=m35$, $p=-1$, $\mathbf{r}=(0,0,0,0,0,0)$, $\mathbf{r}^i=(0,0,0,0,0,0)^i$

$\mathbf{e}_1=\tau^{-2}(1,0,\bar{1},0,\bar{1},\bar{1})^i/2$ $\mathbf{e}_2=\tau^{-2}(1,1,\bar{1},\bar{1},\bar{1},\bar{1})^{i/2}$ $\mathbf{e}_3=\tau^{-2}(1,0,-\tau^{-1},0,0,0)^i$

$\mathbf{e}_4=\tau^{-2}(1,\tau^{-3},\bar{1},\bar{1},\bar{1},\bar{1})^i/2$ $\mathbf{e}_5=\tau^{-2}[(3-\tau^{-2}),0,0,0,0,0]^i/2$

(b) Vectors defining the rhombic triacontahedron (RT) with concave faces [Fig. 3(b)].

(RT) $G_s=m35$, $p=1$, $\mathbf{r}=(0,0,0,0,0,0)$, $\mathbf{r}^i=(0,0,0,0,0,0)^i$

$\mathbf{e}_1=(1,\bar{1},\bar{1},\bar{1},\bar{1},\bar{1})^i/2$ $\mathbf{e}_2=(1,\bar{1},\bar{1},1,\bar{1},\bar{1})^i/2$ $\mathbf{e}_3=(1,\bar{1},\bar{1},0,\bar{1},0)^i/2$

(Concave part on RT) $G_s=mm2$, $p=-1$, $\mathbf{r}=(0,0,0,0,0,0)$, $\mathbf{r}^i=(1,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(0,0,0,\tau^{-3},0,\bar{1})^i/2$ $\mathbf{e}_2=(\tau^{-3},0,\tau^{-2},\tau^{-3}/2,0,-1/2)^i$ $\mathbf{e}_3=(0,0,\tau^{-2},\tau^{-3}/2,0,\bar{1}/2)^i$

(Concave part on RT) $G_s=mm2$, $p=-1$, $\mathbf{r}=(0,0,0,0,0,0)$, $\mathbf{r}^i=(1,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(0,0,0,1,0,\bar{1})^i/2$ $\mathbf{e}_2=(0,0,0,\tau^{-3},0,\bar{1})^i/2$ $\mathbf{e}_3=(0,0,\tau^{-2},1/2,0,\bar{1}/2)^i$

$\mathbf{e}_4=(0,0,\tau^{-2},\tau^{-3}/2,0,\bar{1}/2)^i$ $\mathbf{e}_5=(0,\tau^{-2},\tau^{-2},0,0,0)^i/2$

(c) Vectors defining the rhombic icosahedron (RI) with concave faces [Fig. 3(a)].

(RI) $G_s=5m$, $p=1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$ $\mathbf{r}^i=(0,0,0,0,0,0)^i$

$\mathbf{e}_1=(0,\bar{1},\bar{1},\bar{1},\bar{1},\bar{1})^i/2$ $\mathbf{e}_2=(0,\bar{1},\bar{1},\bar{1},\bar{1},\bar{1})^i/2$ $\mathbf{e}_3=(0,\bar{1},\bar{1},1,\bar{1},1)^i/2$

$\mathbf{e}_4=(0,\bar{1},1,1,\bar{1},1)^i/2$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(\tau^{-3},\tau^{-2},0,\bar{1}/2,0,\tau^{-3}/2)^i$ $e_2=(0,0,0,\bar{1},0,\tau^{-3})^i/2$ $\mathbf{e}_3=(0,\tau^{-2},0,\bar{1}/2,0,\tau^{-3}/2)^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1}/2,\bar{1}/2,0,\bar{1}/2,0)^i$

$\mathbf{e}_1=(0,\tau^{-2},0,\bar{1}/2,0,\tau^{-3}/2)^i$ $\mathbf{e}_2=(0,0,0,\bar{1}/2,0,\tau^{-3}/2)^i$ $\mathbf{e}_3=(0,\tau^{-2},0,\bar{1}/2,0,1/2)^i$

$\mathbf{e}_4=(0,0,0,\bar{1}/2,0,1,2)^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(0,\tau^{-2},0,\bar{1}/2,0,\tau^{-3}/2)^i$ $\mathbf{e}_2=(0,\tau^{-2},0,\bar{1}/2,0,1/2)^i$ $\mathbf{e}_3=(0,\tau^{-2},0,-\tau^{-3}/2,0,1/2)^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(0,\tau^{-2},0,-\tau^{-3}/2,0,1/2)^i$ $\mathbf{e}_2=(0,\tau^{-2},0,\bar{1}/2,0,1/2)^i$ $\mathbf{e}_3=(0,0,0,-\tau^{-3}/2,0,1/2)^i$

$\mathbf{e}_4=(0,0,0,\bar{1},0,1)^i/2$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1},\bar{1},0,\bar{1},0)^i/2$

$\mathbf{e}_1=(0,\tau^{-2},0,-\tau^{-3}/2,-\tau^{-3},\frac{1}{2})^i$ $\mathbf{e}_2=(0,0,0,-\tau^{-3}/2,0,1/2)^i$ $\mathbf{e}_3=(0,\tau^{-2},0,-\tau^{-3}/2,0,\frac{1}{2})^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{r}^i=(0,\bar{1},0,0,\bar{1},1)^i/2$

$\mathbf{e}_1=(0,0,\bar{1}/2,-\tau^{-3}/2,0,0)^i$ $\mathbf{e}_2=(-\tau^{-2},0,\bar{1}/2,-\tau^{-3}/2,-\tau^{-3},0)^i$ $\mathbf{e}_3=(-\tau^{-2},0,\bar{1}/2,-\tau^{-3}/2,0,0)^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$, $\mathbf{R}^i=(0,\bar{1},0,0,\bar{1},1)^i/2$

$\mathbf{e}_1=(0,0,\tau^{-3}/2,1/2,0,0)^i$ $\mathbf{e}_2=(-\tau^{-2},0,\bar{1}/2,-\tau^{-3}/2,-\tau^{-3},0)^i$ $\mathbf{e}_3=(-\tau^{-2},0,\bar{1}/2,-\tau^{-3}/2,0,0)^i$

(Concave part on RI) $G_s=mm2$, $p=-1$, $\mathbf{r}=(\frac{1}{2},0,0,0,0,0)$ $\mathbf{r}^i=(0,\bar{1},0,0,\bar{1},1)^i/2$

$\mathbf{e}_1=(0,0,\bar{1},\bar{1},0,0)^i/2$ $\mathbf{e}_2=(0,0,\bar{1},-\tau^{-3},0,0)^i/2$ $\mathbf{e}_3=(-\tau^{-2},0,\bar{1}/2,\bar{1}/2,0,0)^i$

$\mathbf{e}_4=(-\tau^{-2},0,\bar{1}/2,-\tau^{-3}/2,0,0)^i$ $\mathbf{e}_5=(0,0,\frac{1}{2},\frac{1}{2},0,-\tau^{-2})^i$ $\mathbf{e}_6=(0,0,\tau^{-3},1,0,0)^i/2$

$\mathbf{e}_7=(0,0,1,1,0,0)^i/2$

(d) Vectors defining the D_{1E} dodecahedron (DD) with convex faces [Fig. 3(d)].

(DD) $G_s=m35$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(0,0,0,0,0,0)^i$

$\mathbf{e}_1=(0,0,0,0,\bar{1},0)^i$ $\mathbf{e}_2=(0,0,0,1,\bar{1},0)^i$ $\mathbf{e}_3=(0,0,0,1,\bar{1},1)^i$

(Convex part on DD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(0,0,0,\frac{1}{2},\bar{1},\frac{1}{2})^i$

$\mathbf{e}_1=(-\tau^{-3},0,-\tau^{-2},-\tau^{-3}/2,0,1/2)^i$ $\mathbf{e}_2=(0,0,-\tau^{-2},-\tau^{-3}/2,0,1/2)^i$ $\mathbf{e}_3=(0,0,0,1,0,-\tau^{-3})^i/2$

(Convex part on DD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(0,0,0,\frac{1}{2},\bar{1},\frac{1}{2})^i$

$\mathbf{e}_1=(0,0,0,1,0,\bar{1})^i/2$ $\mathbf{e}_2=(0,-\tau^{-2},0,\frac{1}{2},0,\bar{1}/2)^i$ $\mathbf{e}_3=(0,0,0,\tau^{-3}/2,0,\bar{1}/2)^i$

$\mathbf{e}_4=(0,0,-\tau^{-2},\bar{1}/2,0,\tau^{-3}/2)^i$

TABLE I. (*Continued*).

(Convex part on DD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(0,0,0,\frac{1}{2},\bar{1},\frac{1}{2})^i$
$\mathbf{e}_1=(0,0,-\tau^{-2},\bar{1}/2,0,\tau^{-3}/2)^i$ $\mathbf{e}_2=(0,-\tau^{-2},0,\frac{1}{2},0,\bar{1}/2)^i$ $\mathbf{e}_3=(0,0,-\tau^{-2},-\tau^{-3}/2,0,\frac{1}{2})^i$

(Convex part on DD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(0,0,0,\frac{1}{2},\bar{1},\frac{1}{2})^i$
$\mathbf{e}_1=(0,0,0,1,0,\bar{1})^i/2$ $\mathbf{e}_2=(0,0,0,1,0,-\tau^{-3})^i/2$ $\mathbf{e}_3=(0,-\tau^{-2},0,\frac{1}{2},0,\bar{1}/2)^i$
$\mathbf{e}_4=(0,0,-\tau^{-2},-\tau^{-3}/2,0,\frac{1}{2})^i$

(e) Vectors defining the capped rhombic dodecahedron (CRD) with the edge length of $\tau^{-2}a$ [Fig. 3(e)].

(CRD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(\bar{1},0,1,0,\frac{1}{2},\frac{1}{2})^i$
$\mathbf{e}_1=\tau^{-2}(1,0,\bar{1},0,\bar{1},\bar{1})^i/2$ $\mathbf{e}_2=\tau^{-2}(1,0,\bar{1},0,1,\bar{1})^i/2$ $\mathbf{e}_3=\tau^{-2}(1,0,1,0,1,\bar{1})^i/2$
$\mathbf{e}_4=\tau^{-2}(\frac{1}{2},\tau^{-1},\frac{1}{2},0,\frac{1}{2},\bar{1}/2)^i$

(CRD) $G_s=mm2$ $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(\bar{1},0,1,0,\frac{1}{2},\frac{1}{2})^i$
$\mathbf{e}_1=\tau^{-2}(\bar{1},0,1,0,1,1)^i/2$ $\mathbf{e}_2=\tau^{-2}(\bar{1},0,1,0,1,\bar{1})^i/2$ $\mathbf{e}_3=\tau^{-2}(1,0,1,0,1,\bar{1})^i/2$
$\mathbf{e}_4=\tau^{-2}(\frac{1}{2},\tau^{-1},\frac{1}{2},0,\frac{1}{2},\bar{1}/2)^i$

(CRD) $G_s=mm2$, $p=1$, $\mathbf{r}=(1,1,1,1,1,1)/2$, $\mathbf{r}^i=(\bar{1},0,1,0,\frac{1}{2},\frac{1}{2})^i$
$\mathbf{e}_1=\tau^{-2}(1,0,\bar{1},0,\bar{1},\bar{1})^i$ $\mathbf{e}_2=\tau^{-2}(1,0,1,0,\bar{1},\bar{1})^i/2$ $\mathbf{e}_3=\tau^{-2}(1,0,1,0,1,\bar{1})^i/2$
$\mathbf{e}_4=\tau^{-2}(1,0,1,0,1,1)^i/2$ $\mathbf{e}_5=\tau^{-2}(\bar{1},0,1,0,1,1)^i/2$

method as a Rietveld program used in the refinement of a high-T_c superconducting oxide.[36]

A preliminary refinement showed that B' is negligibly small and the edge-off-center Al,Cu position is fully occupied by Al. Therefore, we neglected the B' factor and fixed the occupation probability of the edge-off-center Al,Cu site in the succeeding calculations. The least-squares refinement converged smoothly at the R factors of 0.076 and 0.085 for 56 x-ray- and 40 neutron diffraction intensities. These are nearly equal to the values obtained by Boissieu *et al.*[23] but, in the present case, the appearance of unacceptable nearest-neighbor distance between the edge-center and edge-off-center positions is avoided by use of the occupation domains described in Sec. II. The observed and calculated diffraction intensities are shown in Figs. 4 and 5. The final parameters are listed in Table II. (Structure-factor tables are available upon request.)

It is noted that Cu occupies preferably the vertex position rather than the edge-center position while the edge-off-center position is completely occupied by either Al or Li. This agrees with the site preference in R-Al-Cu-Li.[33] The model gives a reasonable chemical composition, $Al_{56}Cu_{13}Li_{32}$. (The sample used is $Al_{57}Cu_{11}Li_{32}$.) The point density of the model is $7.629a^{-3}$, which is nearly equal to that of R-Al-Cu-Li, $7.670a^{-3}$. The temperature factor for each atom is almost the same as the corresponding one in a previous analysis[23] except for that of the edge-off-center Al and about twice that of R-Al-Cu-Li.[33] The large temperature factor of the edge-off-center Al corresponds to the displacement of about 0.28 Å. This is consistent with the fact that the displacement of the atom in R-Al-Cu-Li [Al, Cu(4) in Table III] from the ideal position deduced from the above model is particularly large (0.32 Å) (Table III). The result suggests that the edge-off-center Al atoms largely deviates from the assumed position. Thus, the present analysis concludes that the i-Al-Cu-Li quasicrystal has a local atom arrange-

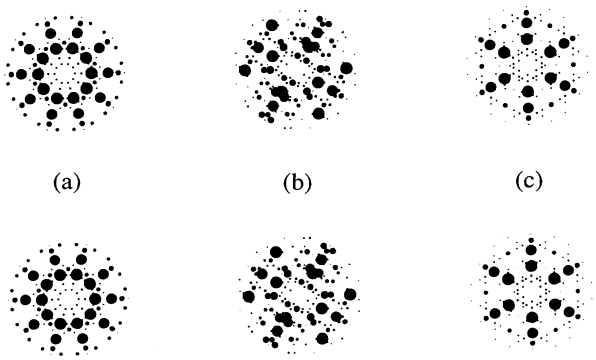

FIG. 4. Observed (upper) and calculated (lower) diffraction patterns for x ray along the (a) fivefold, (b) twofold, and (c) threefold axes.

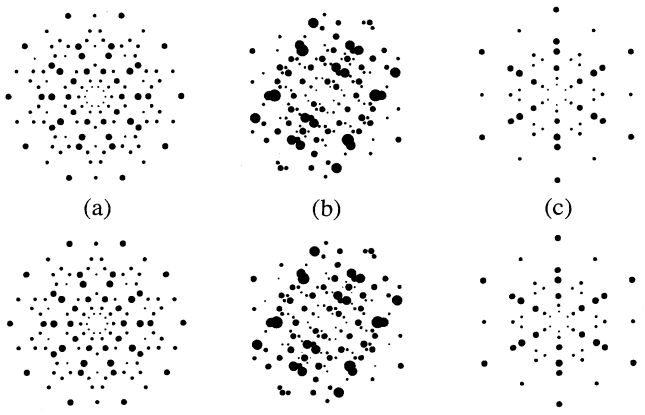

FIG. 5. Observed (upper) and calculated (lower) diffraction patterns for neutron along the (a) fivefold, (b) twofold, and (c) threefold axes.

TABLE II. The temperature factor (B) and occupation probability (p) for each occupation domain (OD). The occupation domains are specified by the labels in Fig. 3. (V, EC, and EOC in the heading mean the vertex, edge-center, and edge-off-center positions.) The standard deviations are in parentheses. Asterisked parameters are fixed.

OD	(b) V	(c) EC	(d) EOC	(e) EOC
B (Å^2)	2.0(2)	1.8(1)	2.6(4)	6(2)
p^{Al}	0.64(8)	0.85(3)		1.0*
p^{Cu}	0.36(8)	0.15(3)		
p^{Li}			1.0*	

ment quite similar to that of the crystal approximant R-Al-Cu-Li.

V. CRYSTAL APPROXIMANTS

As shown by Elser and Kramer,[5,26] an appropriate phason strain or a rotation of the six-dimensional lattice against the external space leads to a periodic crystal structure which is called a crystal approximant for the quasicrystal. The cubic R-Al-Cu-Li is an example of such crystal approximants.[34] There are lots of crystal approximants with several symmetries which are the subgroups of the icosahedral group. In this paper, we consider only cubic structures for the sake of comparison with real crystal approximants. It has been shown that the ideal model mentioned above really leads to the ideal positions close to those of R-Al-Cu-Li.[21] In this section we describe the derivation of such a structure in detail.

The (linear) phason strain is defined by the shear strain between external and internal spaces leaving the internal space invariant. Owing to this property, the shape of the occupation domain is unchanged under the phason strain. The only change is the location of the center of the occupation domain. As a result, the external space cuts across a different position of the occupation domain depending on the strength of the phason strain and this leads to a different structure. The condition of the periodicity is that three linearly independent lattice points in the six-dimensional lattice are on the external space provided that the external space (three-dimensional hyperplane) passes through the origin. Then an infinite number of lattice points are on the external space, forming a three-dimensional periodic structure because of the periodicity of the six-dimensional lattice. Cubic distortion is described by the strain tensor S with $S_{ij}=\delta_{ij}+\phi\delta_{i-3,j}$, where ϕ represents the strength of a cubic phason strain. The external and internal coordinates (with respect to $\mathbf{a}_{0j}$) of the lattice vector $(n_1,n_2,\ldots,n_6)$ are given by $\sum_j M_{ij}^{-1}n_j$ when the phason strain does not exist. The phason strain changes these into $\sum_j (SM^{-1})_{ij}n_j$.

The crystal approximant with the shortest period is obtained when the lattice points $(1,1,1,0,\bar{1},0)$, $(1,0,0,1,1,1)$, and $(0,1,\bar{1},\bar{1},0,1)$ are on the external space. Since both external and internal components of these vectors are mutually orthogonal, the resulting lattice has the cubic symmetry. Then the vector $(1,0,1,1,0,0)$ is also on the external space.[26] Therefore, the lattice is body-centered cubic. The strength of the phason strain in this case is given by $\phi=-\tau^{-3}$. The atom positions in this approximant can be obtained by taking an intersection of the quasicrystal at the external space after deforming the six-dimensional lattice under the phason strain. The coordinates of atoms are listed in Table III together with the experimental values in R-Al-Cu-Li. It is noted that the calculated values are close to observed ones in R-Al-Cu-Li except for the edge-off-center Al,Cu site [Al,Cu(4)].

Another crystal approximant with periods $(1,2,2,0,\bar{1},0)$, $(2,0,0,1,2,1)$, and $(0,1,\bar{1},\bar{2},0,2)$ is obtained when $\phi=\tau^{-5}$. This has a primitive cubic lattice in contrast to the former and its period is τ times longer than that of the former (Table III). Similarly, the lattice points $(n,m,m,0,\bar{n},0)$, $(m,0,0,n,m,n)$, and $(0,n,\bar{n},\bar{m},0,m)$ with Fibonacci numbers m and n are on the external space when $\phi=(m-\tau n)/(m\tau+n)$ and these give a series of cubic structures. We call this the (m,n) structure. The two structures mentioned above are the (1,1) and (2,1) structures of this series. The same procedure can produce an infinite number of cubic approximants for the icosahedral quasicrystal which may be helpful to some theoretical consideration applying the conventional theory to the quasicrystal because their local atom arrangement is quite similar to that of the quasicrystal.

In the remaining part of this section we discuss the structural feature of the (2,1) structure. This is a complicated structure with 651 atoms (440 Al or Cu and 211 Li) in the unit cell provided that the centers of the icosahedral cluster are vacant. In order to simplify a description, we note its framework structure consisting of

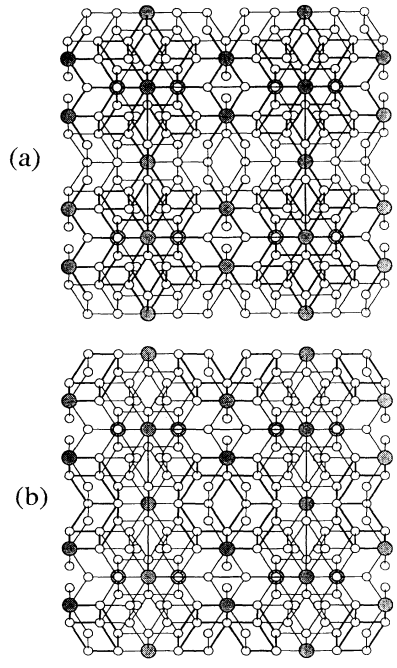

FIG. 6. Projection of the cubic (2,1) structure along the principal axis. The 12-fold vertices are denoted by large circles. The D_{1E} dodecahedron at (a) the origin and rhombic triacontahedron at (b) the body center are indicated by thick lines. Only the vertex positions are drawn.

the vertex positions which are derived from the RT. As in *R*-Al-Cu-Li, the structure includes the 12-fold vertices. They are located at (0,0,0) and $(0,1/2,\tau^{-2}/2)$ and its five equivalent sites under the cubic symmetry (the Wyckoff positions 1*a* and 6*g* in $Pm3$) at which the atom clusters are situated (Fig. 6). At the origin, there is a D_{1E} dodecahedron with the edge length of a [Fig. 1(e), but in this case the structure is in the external space] and a rhombic triacontahedron [Fig. 1(a)] is at the body center of the cubic cell. One 12-fold vertex is at the origin and the other six are on the surface of the unit cell. These two units are connected with six rhombic dodecahedra [Fig. 1(c)] and 30 acute rhombohedra [Fig. 1(d)]. In particular, the 12-fold vertices are connected by the rhombic dodecahedron

TABLE III. The structural parameters of two ideal cubic Al-Cu-Li structures and *R*-Al-Cu-Li. The space groups of the (1,1) and (2,1) structures are $Im3$ and $Pm3$. The 12-fold sites *V* in the (1,1) and *V*(1) and *V*(2) in the (2,1) structures are vacant. The displacements *u* in *R*-Al-Cu-Li are measured from the position of the (1,1) structure. In the (1,1) structure, Al,Cu(1) is at the vertex position, Al,Cu(2) Al,Cu(3) are at the edge-center position and Al,Cu(4) and Li(1)-Li(3) are at the edge-off-center one while the corresponding positions in the (2,1) structure are Al,Cu(1)-Al,Cu(8), Al,Cu(9)-Al,Cu(23), and Al,Cu(24)-Al,Cu(28) and Li(1)-Li(17). [$e=\tau^{-2}/2=0.19098$, $f=(1-\tau^{-2})/2=0.30902$, $g=\tau^{-3}/2=0.11803$, $h=\tau^{-2}=0.38197$, $i=\tau^{-2}/4=0.09549$, $j=(1-\tau^{-2})/4=0.15451$, $k=(1+\tau^{-2})/4=0.34549$, $l=(1-\tau^{-4})/2=0.42705$, $m=\tau^{-4}/2=0.07295$, $n=\tau^{-3}/4=0.05902$, $p=\tau^{-3}=0.23607$, $q=\frac{1}{2}-\tau^{-3}=0.26393$, $r=\frac{1}{2}-\tau^{-2}/4=0.40451$, $s=\frac{1}{2}-\tau^{-3}/4=0.44098$, $t=(1+\tau^{-4})/4=0.28648$, $u=\tau^{-2}-\frac{1}{4}=0.13197$, $v=(1-\tau^{-4})/4=0.21352$, $w=\frac{3}{4}-\tau^{-2}=0.36803$, $x=\tau^{-1}/2+\tau^{-4}=0.45492$, $y=\frac{1}{2}-\tau^{-4}=0.35410$.]

		Al-Cu-Li (1,1)			*R*-Al-Cu-Li			
Atom		*x*	*y*	*z*	*x*	*y*	*z*	*u* (Å)
V	2*a*	0	0	0	0	0	0	0
Al,Cu(1)	24*g*	*f*	0	*e*	0.3150	0	0.1802	0.17
Al,Cu(2)	24*g*	0	*i*	*j*	0	0.0944	0.1544	0.02
Al,Cu(3)	48*h*	*f*	*i*	*k*	0.3104	0.0941	0.3426	0.05
Al,Cu(4)	12*e*	0	$\frac{1}{2}$	*l*	0	$\frac{1}{2}$	0.4037	0.32
Li(1)	12*e*	0	$\frac{1}{2}$	*e*	0	$\frac{1}{2}$	0.1985	0.10
Li(2)	16*f*	*e*	*e*	*e*	0.1874	0.1874	0.1874	0.08
Li(3)	24*g*	0	*f*	*g*	0	0.3047	0.1171	0.06

	Al-Cu-Li (2,1)					Al-Cu-Li (2,1)			
Atom		*x*	*y*	*z*	Atom		*x*	*y*	*z*
V(1)	1*a*	0	0	0	Al,Cu(23)	12*k*	$\frac{1}{4}$	*t*	$\frac{1}{2}$
V(2)	6*g*	0	$\frac{1}{2}$	*e*	Al,Cu(24)	24*l*	*f*	*g*	*p*
Al,Cu(1)	12*j*	*e*	0	*g*	Al,Cu(25)	24*l*	*h*	*m*	*q*
Al,Cu(2)	6*e*	0	*h*	0	Al,Cu(26)	6*g*	*x*	$\frac{1}{2}$	0
Al,Cu(3)	24*l*	*e*	*g*	*f*	Al,Cu(27)	6*h*	$\frac{1}{2}$	$\frac{1}{2}$	*y*
Al,Cu(4)	8*i*	*f*	*f*	*f*	Al,Cu(28)	6*h*	$\frac{1}{2}$	$\frac{1}{2}$	*q*
Al,Cu(5)	12*j*	*h*	*h*	0	Li(1)	12*j*	0	*f*	*g*
Al,Cu(6)	12*k*	*e*	$\frac{1}{2}$	*f*	Li(2)	24*l*	*g*	*h*	*m*
Al,Cu(7)	12*k*	*m*	*e*	$\frac{1}{2}$	Li(3)	8*i*	*g*	*g*	*g*
Al,Cu(8)	12*k*	*h*	$\frac{1}{2}$	*e*	Li(4)	12*j*	*e*	*f*	0
Al,Cu(9)	12*j*	0	*n*	*i*	Li(5)	12*j*	0	*e*	*m*
Al,Cu(10)	24*l*	*e*	*n*	*v*	Li(6)	6*g*	*m*	$\frac{1}{2}$	0
Al,Cu(11)	24*l*	$\frac{1}{4}$	*i*	*g*	Li(7)	24*l*	*h*	*f*	*g*
Al,Cu(12)	12*j*	*n*	*t*	0	Li(8)	6*g*	*f*	$\frac{1}{2}$	0
Al,Cu(13)	12*j*	0	*s*	*i*	Li(9)	24*l*	*l*	*e*	*e*
Al,Cu(14)	24*l*	$\frac{1}{4}$	*v*	*f*	Li(10)	12*k*	$\frac{1}{2}$	*h*	*m*
Al,Cu(15)	24*l*	*n*	*r*	*e*	Li(11)	8*i*	*e*	*e*	*e*
Al,Cu(16)	12*j*	*s*	*t*	0	Li(12)	12*j*	0	*f*	*q*
Al,Cu(17)	12*k*	$\frac{1}{2}$	$\frac{1}{4}$	*i*	Li(13)	6*h*	$\frac{1}{2}$	$\frac{1}{2}$	*g*
Al,Cu(18)	24*l*	*f*	*w*	*r*	Li(14)	24*l*	*h*	*e*	*f*
Al,Cu(19)	24*l*	$\frac{1}{4}$	*r*	*f*	Li(15)	8*i*	*l*	*l*	*l*
Al,Cu(20)	12*k*	*u*	*i*	$\frac{1}{2}$	Li(16)	12*k*	*h*	*f*	$\frac{1}{2}$
Al,Cu(21)	24*l*	*h*	*s*	*i*	Li(17)	1*b*	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
Al,Cu(22)	24*l*	*s*	*r*	*e*					

or the acute rhombohedron as in R-Al-Cu-Li. The appearance of the D_{1E} dodecahedron and the rhombic triacontahedron is characteristic of the (2,1) structure. These are not included in the (1,1) structure or R-Al-Cu-Li but in the 3DPP. The rhombic icosahedron [Fig. 1(b)] appearing in the 3DPP is, however, still absent. The positions of vertices in the rhombic triacontahedron are different from those of the 3DPP because the rhombic triacontahedron appears at the body center and must have the cubic symmetry while it has at most the trigonal symmetry in the 3DPP.

VI. CONCLUDING REMARKS

An ideal structure of the i-Al-Cu-Li quasicrystal was described based on the section method. It contains icosahedral clusters and linking atoms joining them. The clusters are placed at the 12-fold vertices of the 3DPP. The 12-fold vertices are linked with the acute rhombohedra or the rhombic dodecahedra with the same decorations as those of the cubic approximant, R-Al-Cu-Li. It was shown that such an ideal quasicrystal structure can be described by four polyhedral occupation domains placed at the origin, edge center, and body center of the six-dimensional icosahedral lattice. An analytical expression of the structure factor was given for the structure with such polyhedral occupation domains. It includes the symmetry operations explicitly and can calculate the diffraction intensity from the independent part of the domain. A simple method to specify the quasicrystal structure with the use of site symmetry was proposed. By the application of the least-squares program based on the structure-factor formula, the model with four temperature factors and two occupation probabilities was refined to give small-R values (0.076 for x-ray and 0.085 for neutron data). The results showed that the site preference of Al, Cu, and Li atoms is quite similar to that of R-Al-Cu-Li. From the quasicrystal model the structures of two cubic crystal approximants [the (1,1) and (2,1) structures] were derived, one of which is the ideal R-Al-Cu-Li structure and the other is a fictitious one with the lattice constant τ times larger than that of the former.

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APPENDIX

The structure factor of the 3DPP is given by the Fourier integral over the rhombohedra because its occupation domain (rhombic triacontahedron) is divided into two kinds of rhombohedra.[37] A general occupation domain is, however, divided into several tetrahedra instead of rhombohedra as stated in the text. The Fourier integral of the tetrahedron defined by the three vectors $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ is easily calculated with the use of oblique coordinate system: $\mathbf{r}=x_1\mathbf{e}_1+x_2\mathbf{e}_2+x_3\mathbf{e}_3$ and $2\pi\mathbf{q}=q_1\mathbf{e}_1^*+q_2\mathbf{e}_2^*+q_3\mathbf{e}_3^*$, where $\mathbf{e}_1^*$, $\mathbf{e}_2^*$, and $\mathbf{e}_3^*$ are vectors reciprocal to $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$: $\mathbf{e}_i\cdot\mathbf{e}_j^*=\delta_{ij}$. Then $F_0(\mathbf{q})$ is given by

$$\int dV \exp(2\pi i\mathbf{q}\cdot\mathbf{r})=V\int_0^1 dx_1 \exp(iq_1x_1)\int_0^{1-x_1} dx_2 \exp(iq_2x_2)\int_0^{1-x_1-x_2} dx_3 \exp(iq_3x_3)\ ,$$

where V is the volume of the parallelepiped defined by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ and it is used the fact that the volume element dV is given by $Vdx_1dx_2dx_3$. The direct calculation of the above integral leads to Eq. (2) in the text.

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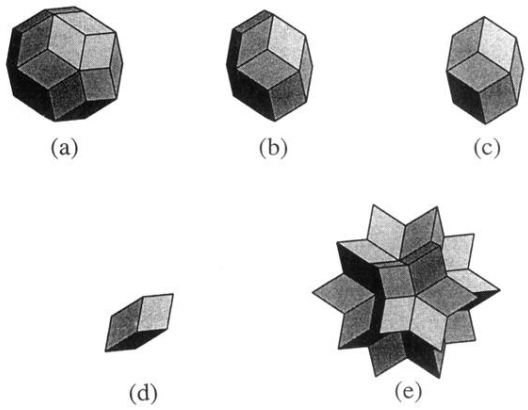

FIG. 1. Occupation domains appearing in the three-dimensional Penrose pattern and its simple decoration. (a) Rhombic triacontahedron, (b) rhombic icosahedron, (c) rhombic dodecahedron, (d) acute rhombohedron, and (e) D_{1E} dodecahedron with the edge length equal to the lattice constant a.

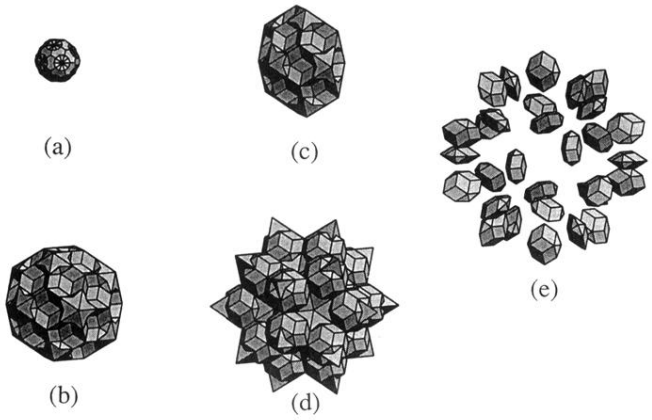

FIG. 3. Occupation domains of the ideal structure for (a) vacant 12-fold, (b) vertex Al,Cu, (c) edge center Al,Cu, (d) edge-off-center Li, and (e) edge-off-center Al,Cu sites. The domain with the shape of (a) is subtracted from the central part of (b) to remove unoccupied 12-fold vertices.

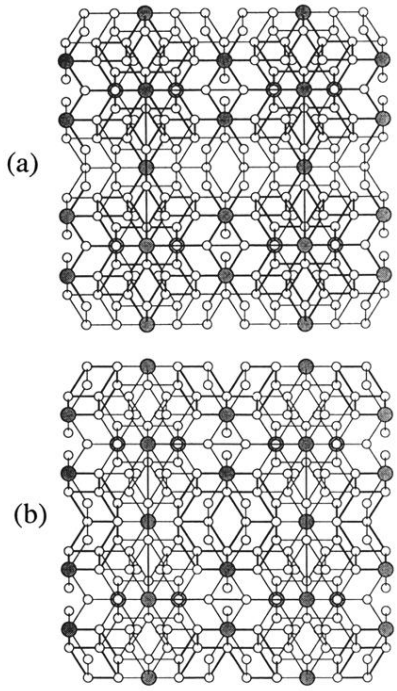

FIG. 6. Projection of the cubic (2,1) structure along the principal axis. The 12-fold vertices are denoted by large circles. The D_{1E} dodecahedron at (a) the origin and rhombic triacontahedron at (b) the body center are indicated by thick lines. Only the vertex positions are drawn.