

### Description of the Dodecagonal Quasicrystal by a Projection Method

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A 2D Ni-Cr quasicrystal displaying a twelfold symmetry consists of a dodecagonal quasi unit cell which is an intergrowth of  $Zr_4Al_3$  and  $Cr_3Si$  structures. If the quasi unit cell is represented by a geometric point, then this quasicrystal can be described by a quasilattice derived by a projection method.

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A number of hexagonal Frank-Kasper phases are known to exist whose structure consists mainly of hexagonal antiprisms or chains of Z14 Kasper polyhedra.<sup>1-4</sup> Electron-diffraction patterns of these phases are characterized by a twelfold distribution of strong diffraction spots, implying a long-range orientational order of these Z14 polyhedra.<sup>5</sup> Ishimasa, Nissen, and Fukano<sup>6</sup> have recently reported an electron-diffraction pattern displaying a twelfold symmetry but no translational symmetry in evaporated Ni-Cr films. They have correctly reached the following two conclusions: (1) A two-dimensional twelfold Ni-70.6 at.% Cr quasicrystal consists of two basic constituents, i.e., the  $Cr_3Si$  and  $Zr_4Al_3$  units, both having the basic edge length of 4.58 Å as measured by Yukawa *et al.*<sup>7</sup> (2) The high-resolution image of these Ni-Cr particles can be explained by a model of interlinked regular dodecagons. However, they did not give the detailed arrangement of the atoms in each dodecagon and how these dodecagons were linked together. We propose a preliminary solution of these problems first by deriving a twelfold quasilattice from a projection method.

We now define vectors  $q_1^{\parallel}, q_2^{\parallel}, \dots, q_6^{\parallel}$ , each of which starts from the origin and ends at a vertex of a regular dodecagon as shown in Fig. 1, as the projections of the basic vectors  $a_1, a_2, \dots, a_6$ , respectively, of a 6D cubic

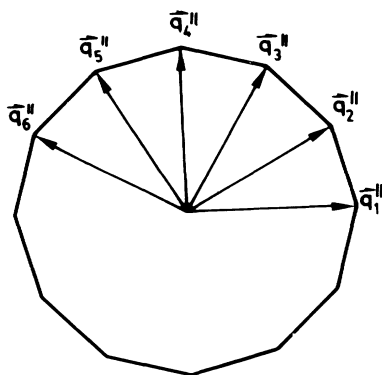


FIG. 1. Quasibasic vectors  $q_1^{\parallel}, q_2^{\parallel}, \dots, q_6^{\parallel}$  of a dodecagonal quasicrystal.

crystal into a 2D subspace. Vectors  $q_1^{\perp}, q_2^{\perp}, \dots, q_6^{\perp}$  represent the projections of  $a_1, a_2, \dots, a_6$  into a 4D subspace perpendicular to the 2D subspace. Defining

$$Q^{\parallel} = \begin{pmatrix} q_1^{\parallel} \\ q_2^{\parallel} \\ q_3^{\parallel} \\ q_4^{\parallel} \\ q_5^{\parallel} \\ q_6^{\parallel} \end{pmatrix}, \quad Q^{\perp} = \begin{pmatrix} q_1^{\perp} \\ q_2^{\perp} \\ q_3^{\perp} \\ q_4^{\perp} \\ q_5^{\perp} \\ q_6^{\perp} \end{pmatrix}, \quad A = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix},$$

we have  $Q^{\parallel} = P^{\parallel}A$ ,  $Q^{\perp} = P^{\perp}A$ ,  $P^{\parallel}P^{\parallel} = P^{\parallel}$ , and  $P^{\perp}P^{\perp} = P^{\perp}$ , where

$$P^{\parallel} = \frac{1}{6} \begin{pmatrix} 2 & \sqrt{3} & 1 & 0 & \bar{1} & \sqrt{3} \\ \sqrt{3} & 2 & \sqrt{3} & 1 & 0 & \bar{1} \\ 1 & \sqrt{3} & 2 & \sqrt{3} & 1 & 0 \\ 0 & 1 & \sqrt{3} & 2 & \sqrt{3} & 1 \\ \bar{1} & 0 & 1 & \sqrt{3} & 2 & \sqrt{3} \\ \sqrt{3} & \bar{1} & 0 & 1 & \sqrt{3} & 2 \end{pmatrix}$$

and  $P^{\perp} = I - P^{\parallel}$ ;  $I$  is the unit matrix. Suppose  $r$  represents the lattice vector of the 6D cube; then

$$r = \tilde{M}A,$$

where  $\tilde{M} = [m_1, m_2, \dots, m_6]$ ;  $m_i$  ( $i = 1, 2, \dots, 6$ ) are integers. If we use  $r_p^{\parallel}$  and  $r_p^{\perp}$  for the projections of  $r$  in the parallel and orthogonal subspaces, respectively, we have

$$r_p^{\parallel} = \tilde{M}Q^{\parallel} = \tilde{M}P^{\parallel}A, \tag{1}$$

and

$$r_p^{\perp} = \tilde{M}P^{\perp}A.$$

$r_p^{\parallel}$  was calculated from the formula (1) under the constraint  $|r_p^{\perp}| \leq \beta a$  or  $\tilde{M}P^{\perp}A \leq \beta^2$ , where  $a = |a_i|$  ( $i = 1, 2, \dots, 6$ ). The result showed that the end points of  $r_p^{\parallel}$  formed a dodecagonal quasilattice [see Fig. 2(a)] whose configuration depends on  $\beta$ . Let  $\beta = \gamma[(2 + \sqrt{3})^{1/2}]^n$  ( $n$  is an integer and  $\gamma$  is a real number arbitrarily chosen); then  $\gamma$  determines the shape of the quasi-

lattice and  $n$  the scale. Thus for constant  $\gamma$  but different variable  $n$ , similar quasilattices result, the only difference being the edge length of the smallest dodecagon. For example, the edge length of the smallest dodecagon increases  $(2+\sqrt{3})^{1/2}$  times when  $n$  decreases by 1. If we keep  $n$  constant and change  $\gamma$  from 1 to  $(2+\sqrt{3})^{1/2}$ , the structure will change from that corresponding to  $[(2+\sqrt{3})^{1/2}]^n$  to that corresponding to  $[(2+\sqrt{3})^{1/2}]^{n+1}$  continuously. This indicates that the dodecagonal quasilattice has self-similarity. Gardner,<sup>8</sup> Bruijn,<sup>9</sup> Dekking,<sup>10</sup> and others have pointed out the self-similarity and inflation rules of Penrose and other aperiodic tilings. By this criterion, our model is also a kind of Penrose tiling. Bruijn<sup>9</sup> and others pointed out that the structure can be described in terms of Penrose tiling or by a projection method and that these two approaches are equivalent to each other. The dodecagonal quasilattice is a projection onto a 2D subspace from a 6D hyperspace and, therefore, it is a 2D quasilattice.

Figure 2 shows a quasilattice corresponding to  $\beta = 1.838[(2+\sqrt{3})^{1/2}]^{-1}$ . This quasilattice is characterized by interlinked regular dodecagons. The edge length of the dodecagon may be determined by indexing of the electron diffraction spots of the quasicrystal. The electron diffraction spots are also the projection of a 6D reciprocal cubic lattice onto a 2D reciprocal subspace and have the self-similarity which causes difficulty in indexing. However, as Elser<sup>11</sup> pointed out, diffraction spots can be indexed in accordance with their intensity. If we ignore the effect of the atomic distribution in a quasi unit cell, as a first-order approximation, the intensity will depend on the lengths of  $\mathbf{g}^{\parallel}$  and  $\mathbf{g}^{\perp}$  which can be calculated by the following formulas:

$$|\mathbf{g}^{\parallel}| = (\tilde{H}P^{\parallel}H)^{1/2} |\mathbf{a}^*|,$$

$$|\mathbf{g}^{\perp}| = (\tilde{H}P^{\perp}H)^{1/2} |\mathbf{a}^*|,$$

where  $\tilde{H} = (h_1, h_2, \dots, h_6)$  and is the index of a 6D reciprocal lattice point and  $h_i$  ( $i=1, 2, \dots, 6$ ) are integers. Roughly speaking, the smaller  $|\mathbf{g}^{\parallel}|$  and  $|\mathbf{g}^{\perp}|$  of a reciprocal spot are, the stronger its  $I_g$  is. Our calculation showed that for  $|\mathbf{g}^{\parallel}|/|\mathbf{a}^*|$  (i.e.,  $\alpha^{\parallel}$ )  $\leq 3.732$  and  $|\mathbf{g}^{\perp}|/|\mathbf{a}^*|$  (i.e.,  $\alpha^{\perp}$ )  $\leq 0.5176$  there were only two groups of diffraction spots, i.e.,  $\{001111\}$  and  $\{012221\}$  (see Table I). [ $(h_1, h_2, \dots, h_6)$  represents a single diffraction spot,  $\{h_1, h_2, \dots, h_6\}$ , twelve spots symmetrically distributed about a twelvefold axis.] Figure 3 shows the distribution and indices of these spots which happen to be those that are detectable in Fig. 1(b) of Ref. 6.

The lengths  $|\mathbf{a}^*|$  and  $|\mathbf{g}|$  of basic vectors of a 6D reciprocal cube lattice and of a quasilattice can be calculated by

$$|\mathbf{a}^*| = |\mathbf{g}^{\parallel}|/\alpha^{\parallel},$$

$$|\mathbf{q}| = 0.57735 |\mathbf{a}| = 0.57735 \alpha^{\parallel} / |\mathbf{g}^{\parallel}|,$$

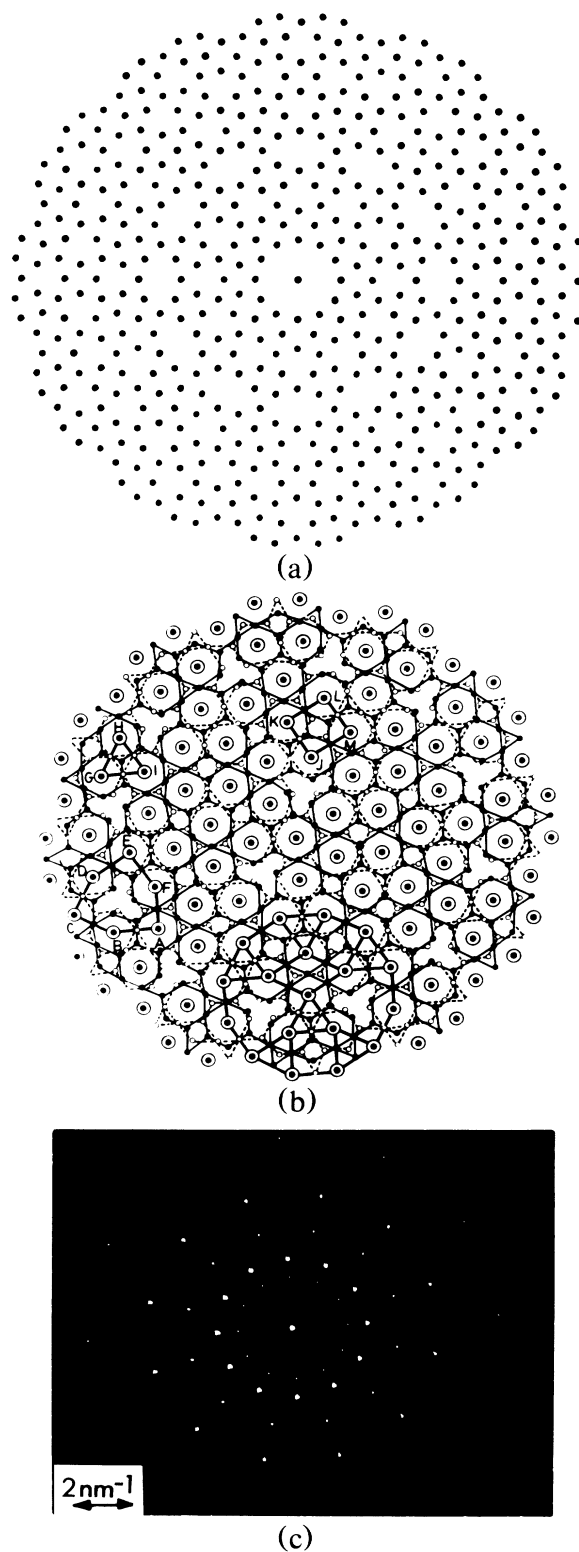


FIG. 2. (a) A quasilattice of a dodecagonal quasicrystal. (b) Atomic structure of Ni-Cr dodecagonal quasicrystal. (c) Optical diffraction of a much bigger dodecagonal quasilattice than (a).

TABLE I. Calculated  $|\mathbf{g}^{\parallel}|/|\mathbf{a}^*|$  and  $|\mathbf{g}^{\perp}|/|\mathbf{a}^*|$  for 6D reciprocal cubic lattice spots  $\{h_1, h_2, \dots, h_6\}$ .

$\{h_1 h_2 h_3 h_4 h_5 h_6\}$	$\alpha^{\parallel} ( \mathbf{g}^{\parallel} / \mathbf{a}^* )$	$\alpha^{\perp} ( \mathbf{g}^{\perp} / \mathbf{a}^* )$
012221	3.732	0.2679
001111	1.932	0.5179
011111	2.155	0.5977
210 $\bar{1}\bar{1}\bar{2}$	3.244	0.6859
2110 $\bar{1}\bar{1}$	1.577	0.7155

where  $\mathbf{g}^{\parallel}$  can be measured by an experiment, while  $\alpha^{\parallel}$  can be found from Table I. According to Fig. 1(b) of Ref. 6,  $|\mathbf{g}^{\parallel}|$  of (012221) was measured to be 5.02 nm<sup>-1</sup>. From the above equations, we have

$$|\mathbf{a}^*| = 1.345 \text{ nm}^{-1}, \quad |\mathbf{a}| = 0.743 \text{ nm},$$

$$|\mathbf{q}| = 0.429 \text{ nm},$$

where  $|\mathbf{q}|$  is in an agreement with the result reported by Yukama *et al.*<sup>7</sup> with a difference of 6%. Finally, a structure having a twelvefold symmetry is constructed by replacing each quasilattice point by one quasi unit cell (QUC) which is described below.

The quasi unit cell of a twelvefold quasicrystal is indicated in Fig. 2(b) by a regular dodecagon of thick lines. The twelve vertices of the dodecagon together with the six dots inside it, which are all located at the centers of corresponding hexagonal antiprisms due to the intergrowth of Zr<sub>4</sub>Al<sub>3</sub> and Cr<sub>3</sub>Si units, form a framework of the unit cell. The square JKLM is the Cr<sub>3</sub>Si unit, the regular triangle HGI, a half of the Zr<sub>4</sub>Al<sub>3</sub> unit, while the hexagon ABCDEF is three incomplete Cr<sub>3</sub>Si units having a threefold symmetry which has already been observed by Ishimasa, Nissen, and Fukano<sup>6</sup> inside a dodecagon in the high-resolution image of their Ni-Cr quasicrystal. It can be seen in Fig. 2(b) that there are three Cr<sub>3</sub>Si units, eight triangles representing the eight halves of Zr<sub>4</sub>Al<sub>3</sub> units, and two hexagons showing a threefold symmetry in a QUC. This QUC, like the unit cells of Cr<sub>3</sub>Si, Zr<sub>4</sub>Al<sub>3</sub>, and other hexagonal Frank-Kasper phases, consists of four layers. The double circles are at the  $\frac{1}{4}$  and  $\frac{3}{4}$  levels, respectively, while the circles connected by dotted lines are at the Z=0 level and the small dots connected by full lines at the Z= $\frac{1}{2}$  level, forming hexagonal antiprisms.

The structure of a two-dimensional quasicrystal having a twelvefold symmetry can be obtained by placing one QUC described above on each quasilattice point.

Figure 2(b) indicates the following distinctions between a QUC of a twelvefold quasicrystal and a 2D unit cell of a crystal: (1) The former is a regular dodecagon in the two-dimensional space, whereas the latter is a parallelogram. (2) The former has no translational symmetry, but has rotational symmetry. (3) Unlike the latter, the former cannot fill the whole space by simple translational operations without overlapping. However,

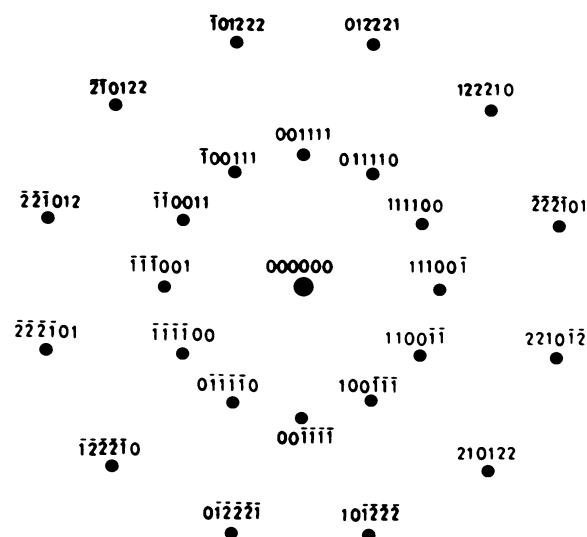


FIG. 3. The distribution and indices of two group diffraction spots,  $\{001111\}$  and  $\{012221\}$ , of a dodecagonal quasilattice.

in the overlapped area the atoms of one unit cell exactly coincide with those of the others. (4) The former has twelve possible orientations, whereas the latter has only one.

The model of quasilattice proposed in the present paper is quite a general one which can be applied for the description of any twelvefold quasicrystal, though the model for the atomic structure is based on a specific Ni-70.6 at.% Cr material. This is quite similar in spirit to such a situation, as the Penrose tiling<sup>12</sup> is well suited for any fivefold quasicrystal lattice, while a specific atomic structure only corresponds to a fivefold quasicrystal with a specific composition.<sup>13-15</sup>

Figure 2(c) shows a typical optical diffraction pattern of a much bigger dodecagonal quasilattice than Fig. 2(a). Obviously, the spots in Fig. 2(c) cannot be defined by any parallelogram. The strong spots are consistent with those in Fig. 1(b) of Ref. 6 while the weak ones do not appear in that figure. This may be because Fig. 2(c) is the optical transformation of an ideal quasilattice, whereas Fig. 1(b) of Ref. 6 is that of a high-resolution image with many imperfections. The scale of Ref. 2(c) was calculated according to  $|\mathbf{q}| = 0.458 \text{ nm}$ .

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