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Solving a 3-dimensional quasicrystal structure in 6-dimensional space using the direct method

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Dedicated to Professor Dr. M. M. Woolfson on the occasion of his 65th birthday

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Abstract. A direct method was tested in solving the structure of a 3-dimensional quasicrystal in 6-dimensional space. Theoretical 3-dimensional diffraction data were used which contain Gaussian distribution errors with a mean error of about 20% for intensities. The diffraction data were firstly converted to a set of 6-dimensional structure factors. The window function used for the conversion was measured from the Patterson origin peak in pseudo space. A direct method was then applied to solve the phase problem in 6-dimensional space. Test results showed that the procedure is very efficient.

1. Introduction

The discovery of icosahedral phases in rapidly quenched Al–Mn alloy (Shechtman et al., 1984) brought about a great deal of interest in the structural characteristics of these phases. Since then, various structure models for quasicrystals have been put forth. Because of the nonperiodicity, it is very difficult to determine the atomic positions in a quasicrystal in physical space using conventional methods. Elser (1986) showed that the three-dimensional (3D) Penrose tiling having the icosahedron symmetry can be obtained by projecting a subset of six-dimensional (6D) lattice on a special 3D hyperplane $E_{\parallel}$. This method has been widely accepted to describe quasicrystal structures. 6D structure models have been set up for several icosahedral quasicrystals such as $(Al,Zn)_{49}Mg_{33}$ (Elser and Henley, 1985; Henley and Elser, 1986), (Al,Si)–Mn (Cahn, Gratias and Mozer, 1988) and Al_6CuLi_3 (Pan, Cheng and Li, 1990). All of them are simple periodic

structures in 6D space. This provides the possibility that a quasicrystal structure can be determined by solving firstly the corresponding structure in 6D space and then converting the result into 3D space (de Boissieu, Janot and Dubois et al., 1991; Cornier-Quiquandon, Quivy and Lefebvre et al., 1991). Li, Wang and Fan (1987) and Xiang, Li and Fan (1990) have proposed a procedure for this purpose by using the direct method. With this procedure, the 3D diffraction data of a quasicrystal are first converted into 6D space. Then a multi-dimensional direct method is used to derive phases for the 6D reflections. Finally the 6D E-map is cut with a 3D hyperplane to obtain the 3D quasicrystal structure. So far the method has been only tested with a 1D Fibonacci sequence. Before the method can be used in practice, further test with higher dimensional model is necessary. Here we present the results on a thorough test with the 3D model of the quasicrystal of Al_6CuLi_3.

2. Method

2.1. Representing a quasicrystal in multi-dimensional space

According to the 'cut method' originally proposed by de Wolff (1974) for the description of incommensurate modulated structures, a 3D quasicrystal can be considered as a 6D periodic structure cut with a 3D hyperplane. A simple formulation for this purpose was described by Li and Cheng (1990) which is reviewed briefly in the following.

A 6D lattice function in real space is constructed by a series of delta functions arranged at the positions of lattice points, we write

$$L_0(\mathbf{r}_\parallel,\mathbf{r}_\perp) = \sum_{\mathbf{R}_\parallel}\sum_{\mathbf{R}_\perp}\delta(\mathbf{r}_\parallel-\mathbf{R}_\parallel)\delta(\mathbf{r}_\perp-\mathbf{R}_\perp). \tag{1}$$

Here $\mathbf{r}_\parallel(x_\parallel,y_\parallel,z_\parallel)$ and $\mathbf{r}_\perp(x_\perp,y_\perp,z_\perp)$ denote coordinate vectors, while $\mathbf{R}_\parallel$ and $\mathbf{R}_\perp$ denote lattice vectors in physical and pseudo space respectively. Axes $x_\parallel$, $y_\parallel$, $z_\parallel$, $x_\perp$, $y_\perp$ and $z_\perp$ are generally not parallel to the basic vectors of the 6D unit cell. Consider a special 6D lattice $L(\mathbf{r}_\parallel,\mathbf{r}_\perp)$, which is obtained by the convolution of L_0 with a window function:

$$W(\mathbf{r}_\perp) = \begin{cases} 1, & \text{inside a certain region in the pseudo space} \\ 0, & \text{elsewhere} \end{cases}.$$

We thus have

$$L(\mathbf{r}_\parallel,\mathbf{r}_\perp) = W(\mathbf{r}_\perp) * L_0(\mathbf{r}_\parallel,\mathbf{r}_\perp), \tag{2}$$

where $*$ denotes the convolution operation. The reciprocal of L is then

$$\Omega(\mathbf{h}_\parallel,\mathbf{h}_\perp) = S(\mathbf{h}_\perp)\Omega_0(\mathbf{h}_\parallel,\mathbf{h}_\perp), \tag{3}$$

where $S(\mathbf{h}_\perp)$ and $\Omega_0(\mathbf{h}_\parallel,\mathbf{h}_\perp)$ are the Fourier transform of $W(\mathbf{r}_\perp)$ and $L_0(\mathbf{r}_\parallel,\mathbf{r}_\perp)$ respectively. It is obvious that L and Ω are quite different in the shape and size of their lattice nodes and in their boundary conditions. The lattice L is unlimited, its lattice nodes have definite size and shape in the pseudo space but they are sharp (delta-function like) in the physical space. On the other hand, the reciprocal lattice Ω is limited and its lattice nodes are sharp in both physical and pseudo spaces. Now a 3D quasilattice $q(\mathbf{r}_\parallel)$ can be obtained by cutting a 6D lattice L with the 3D physical space. For example, if $L(\mathbf{r}_\parallel,\mathbf{r}_\perp)$ is a 6D cubic lattice with the window function corresponding to a triacontahedron, then by cutting L with the 3D physical space, we get a quasilattice $q(\mathbf{r}_\parallel)$ equal to a standard 3D Penrose tiling. Since Fourier transforming a section of a function is equivalent to projecting the Fourier transform of that function along the direction perpendicular to the section, the Fourier transform of $q(\mathbf{r}_\parallel)$ will be

$$Q(\mathbf{h}_\parallel) = \int \Omega(\mathbf{h}_\parallel,\mathbf{h}_\perp)\mathrm{d}\mathbf{h}_\perp = \sum_{\mathbf{H}_\parallel} \sum_{\mathbf{H}_\perp} S(\mathbf{H}_\perp)\delta(\mathbf{h}_\parallel - \mathbf{H}_\parallel), \tag{4}$$

where $\mathbf{H}_\parallel$ and $\mathbf{H}_\perp$ are the components of 6D reciprocal lattice vectors in the physical and pseudo space respectively. The inverse Fourier transform of Equation (4) gives the formula for quasilattice identical to the density wave expression:

$$q(\mathbf{r}_\parallel) = \sum_{\mathbf{H}_\parallel} \sum_{\mathbf{H}_\perp} S(\mathbf{H}_\perp)\mathrm{e}^{-i2\pi\mathbf{H}_\parallel\cdot\mathbf{r}_\perp}. \tag{5}$$

The relationship among L_0, Ω_0, L, Ω, q and Q is summarized as in Figure 1. Based on the above description, we can now set up the relationship between a 3D quasicrystal structure and the corresponding 6D regular periodic structure. A 6D regular periodic structure is constructed by the convolution of the lattice L_0 with the atomic arrangement in a unit cell, $\varrho(\hat{\mathbf{r}})$, which is represented by the electron density distribution in X-ray diffraction or the potential distribution in electron diffraction. By replacing L_0 in Figure 1 with $\varrho(\hat{\mathbf{r}})*L_0$ and following the relationships given in Figure 1 we obtain a similar diagram Figure 2 showing the relationship between a 3D quasicrystal and the corresponding 6D periodic structure.

2.2. Structure analysis in multi-dimensional space

An atom in a 6D regular periodic structure can be defined such that the intersection of which with the physical space gives a real atom, while the intersection with the pseudo space gives a delta function, i.e.

$$\varrho_j(\mathbf{r}_\parallel,\mathbf{r}_\perp) \equiv \varrho_j(\mathbf{r}_\parallel)\delta(\mathbf{r}_\perp). \tag{6}$$

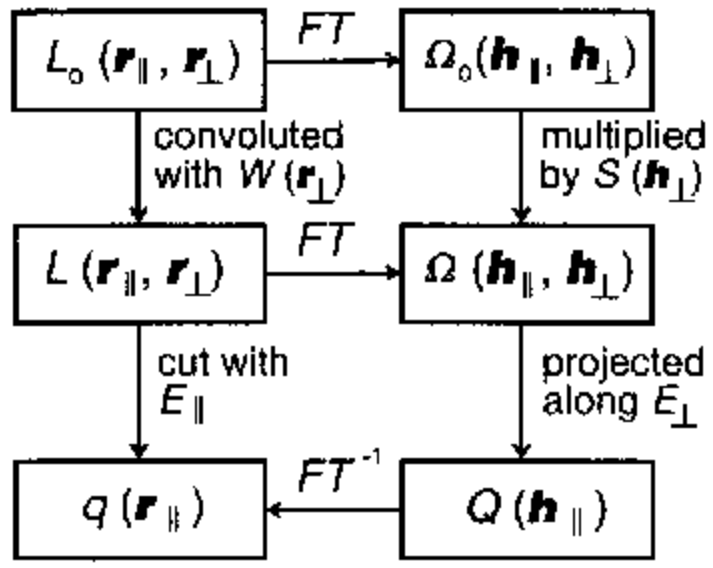


Fig. 1. Schematic diagram showing the principle of deriving the quasiperiodic lattice function in the cut description. L_0 is a 6D periodic lattice. L is a special 6D periodic lattice with its nodes elongated in pseudo space. q is the quasiperiodic lattice cut from L. Ω_0, Ω and Q are the Fourier transform of L_0, L and q respectively. FT stands for Fourier transform. FT^{-1} stands for inverse FT. $E_\parallel$ stands for the physical space. $E_\perp$ stands for the pseudo space.

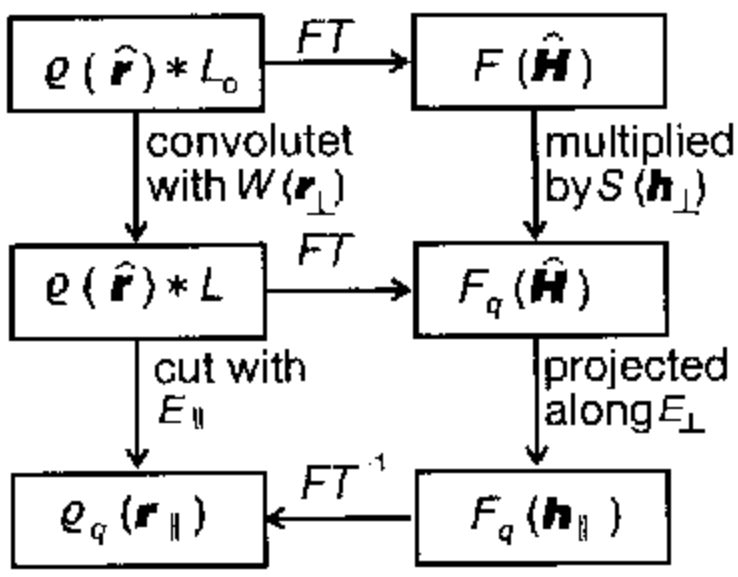


Fig. 2. Schematic diagram showing the relationship between a 3D quasicrystal structure and the corresponding 6D periodic structure. $\varrho_q(\mathbf{r}_\parallel)$ is a 3D quasicrystal structure. $\varrho(\hat{\mathbf{r}})*L$ is a special 6D periodic structure corresponding to $\varrho_q(\mathbf{r}_\parallel)$ with its atoms spread in pseudo space according to the window function $W(\mathbf{r}_\perp)$. $\varrho(\hat{\mathbf{r}})*L_0$ is a 6D regular periodic structure. $F(\hat{\mathbf{H}})$ is the structure factor of $\varrho(\hat{\mathbf{r}})*L_0$. $F_q(\hat{\mathbf{H}})$ and $F_q(\mathbf{h}_\parallel)$ are the structure factors of the quasicrystal represented in 6D and 3D space respectively.

The atomic scattering factor can thus be defined as the same of the corresponding 3D real atom

$$f_j(\mathbf{h}_\parallel, \mathbf{h}_\perp) = f_j(\mathbf{h}_\parallel). \tag{7}$$

Accordingly the structure factor of $\varrho(\hat{\mathbf{r}})*L_0$ is

$$F(\hat{\mathbf{H}}) = \sum_{j=1}^{N} f_j(\mathbf{H}_\parallel) e^{i2\mu\hat{\mathbf{H}}\cdot\hat{\mathbf{r}}_j}, \tag{8}$$

while the structure factor of $\varrho(\hat{\mathbf{r}})*L$ is

$$F_q(\hat{\mathbf{H}}) = \sum_{j=1}^{N} S(\mathbf{H}_\perp) f_j(\mathbf{H}_\parallel) e^{i2\pi \hat{\mathbf{H}} \cdot \hat{\mathbf{r}}_j}. \tag{9}$$

Here $\hat{\mathbf{H}}$ is a lattice vector of the 6D reciprocal lattice Ω_0, $\hat{\mathbf{r}}_j$ is the 6D coordinate vector of the j^{th} 6D atom. Since Ω_0 is a regular 6D periodic reciprocal lattice, $\hat{\mathbf{H}}$ can be expressed in terms of the basis vectors of Ω_0. We have

$$\hat{\mathbf{H}} = \sum_{i=1}^{6} h_i \mathbf{b}_i, \tag{10}$$

where $\mathbf{b}_i$'s are the basis vectors of Ω_0, h_i's are the six components of $\hat{\mathbf{H}}$ in the directions of $\mathbf{b}_i$'s, they are also the six integer indices of the diffraction spot at the end of $\hat{\mathbf{H}}$. On the other hand, by a coordinate transform, $\hat{\mathbf{H}}$ can be split into two components $\mathbf{H}_\parallel$ and $\mathbf{H}_\perp$. Both $\mathbf{H}_\parallel$ and $\mathbf{H}_\perp$ do not have simple indices. Similarly a coordinate vector $\hat{\mathbf{r}}$ in the regular 6D periodic lattice L_0 can be written as

$$\hat{\mathbf{r}} = \sum_{i=1}^{6} x_i \mathbf{a}_i, \tag{11}$$

where $\mathbf{a}_i$'s are the basis vectors of L_0, x_i's are the components of $\hat{\mathbf{r}}$ in the directions of $\mathbf{a}_i$'s. $\hat{\mathbf{r}}$ can also be split into the components in 3D physical space and 3D pseudo space i.e. $\mathbf{r}_\parallel$ and $\mathbf{r}_\perp$ respectively. By inverse Fourier transform of Equation (8), we have

$$\varrho_0(\hat{\mathbf{r}}) = \varrho(\hat{\mathbf{r}})*L_0 = \frac{1}{V}\sum_{\hat{\mathbf{H}}} F(\hat{\mathbf{H}}) e^{-i2\pi \hat{\mathbf{H}} \cdot \hat{\mathbf{r}}}, \tag{12}$$

where V is the volume of the 6D unit cell of L_0. Equations (8) and (12) provide the basis of structure analysis of quasicrystals, since traditional methods for crystal structure analysis can easily be extended from 3D space to higher-dimensional space. As an example, direct methods have been successfully extended to multi-dimensional space and used to solve incommensurate modulated structures (Hao, Liu and Fan, 1987). In order to use direct methods to solve quasicrystal structures, the main problem is to obtain a set of structure factor magnitudes $|F(\hat{\mathbf{H}})|$ (see Fig. 2). Our starting point is at the lower-right corner of Figure 2, i.e. a set of $|F_q(\mathbf{H}_\parallel)|$ which can be derived from the diffraction intensities of the quasicrystal. By indexing all the observed reflections with six integer indices we obtain a set of $|F_q(\hat{\mathbf{H}})|$ in 6D space. Now before we can convert $|F_q(\hat{\mathbf{H}})|$ to $|F(\hat{\mathbf{H}})|$ we need the knowledge of the shape function $S(\mathbf{H}_\perp)$ (see Equations (8) and (9)). This can be achieved by inspecting the inverse Fourier transform of $|F_q(\hat{\mathbf{H}})|^2$, the Patterson function of the quasicrystal (Xiang, Li and Fan, 1990).

According to Equations (8) and (9), if in the pseudo space all the atoms have the same shape function $S(\mathbf{H}_\perp)$ we can write

$$F_q(\hat{\mathbf{H}}) = S(\mathbf{H}_\perp)F(\hat{\mathbf{H}}). \tag{13}$$

Thus we have by the convolution theorem

$$\begin{aligned} P_q(\hat{\mathbf{r}}) &= P_q(\mathbf{r}_\parallel,\mathbf{r}_\perp) = FT^{-1}[|F_q(\hat{\mathbf{H}})|^2] \\ &= P(\mathbf{r}_\parallel,\mathbf{r}_\perp)*[W(\mathbf{r}_\perp)*W(\mathbf{r}_\perp)], \end{aligned} \tag{14}$$

where $P(\mathbf{r}_\parallel,\mathbf{r}_\perp)$ is the inverse Fourier transform of $|F(\hat{\mathbf{H}})|^2$, i.e. the Patterson function of $\varrho_0(\hat{\mathbf{r}})$. Our task is to find the boundary of $W(\mathbf{r}_\perp)$. Consider a region near $\mathbf{r}_\perp = 0$ on the section at $\mathbf{r}_\parallel = 0$, $P(0,\mathbf{r}_\perp)$ will be a delta function centered on $\mathbf{r}_\perp = 0$. Hence within a region near the origin, we can write

$$P_q(0,\mathbf{r}_\perp) = \text{constant} \times W(\mathbf{r}_\perp)*W(\mathbf{r}_\perp). \tag{15}$$

$W(\mathbf{r}_\perp)*W(\mathbf{r}_\perp)$ has a maximum at $\mathbf{r}_\perp = 0$. It gradually falls to zero, or in practice falls to a base level, as $|\mathbf{r}_\perp|$ increases to a value equal to the width of $W(\mathbf{r}_\perp)$ in the direction of $\mathbf{r}_\perp$. Hence we can determine the boundary of $W(\mathbf{r}_\perp)$ from the shape of the Patterson origin peak. Once the boundary of $W(\mathbf{r}_\perp)$ and so the shape function $S(\mathbf{H}_\perp)$ has been found, a set of $|F(\hat{\mathbf{H}})|$ can then be obtained from $|F_q(\hat{\mathbf{H}})|$. By solving the phase problem for $|F(\hat{\mathbf{H}})|$ with direct methods, the structure $\varrho_0(\hat{\mathbf{r}})$ is resulted. Finally the quasicrystal structure $\varrho_q(\mathbf{r}_\parallel)$ is obtained from $\varrho_0(\hat{\mathbf{r}})$ by the cut method.

3. The model

The icosahedral quasicrystal T2$-$$Al_6CuLi_3$ can be obtained from a 6D hypercubic crystal with lattice constant $a = 7.146$ Å, and 27 atoms inside the 6D unit cell (Pan, Cheng and Li, 1990). The superspace group is $P\bar{5}3m$ (Janssen, 1986), with the 6D generators of the corresponding point group given by

$$\Gamma(\alpha) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Gamma(\beta) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{16}$$

$$\Gamma(\gamma) = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

The three independent atomic sites and their 6D parameters are listed in Table 1. An overall temperature factor ($B = 1.0$ Å^2) was assumed. The relationship between the 6D coordinates and the coordinates in 3D physical and 3D pseudo space is given in the Appendix.

Table 1. The structure parameters of the 6D crystal model.

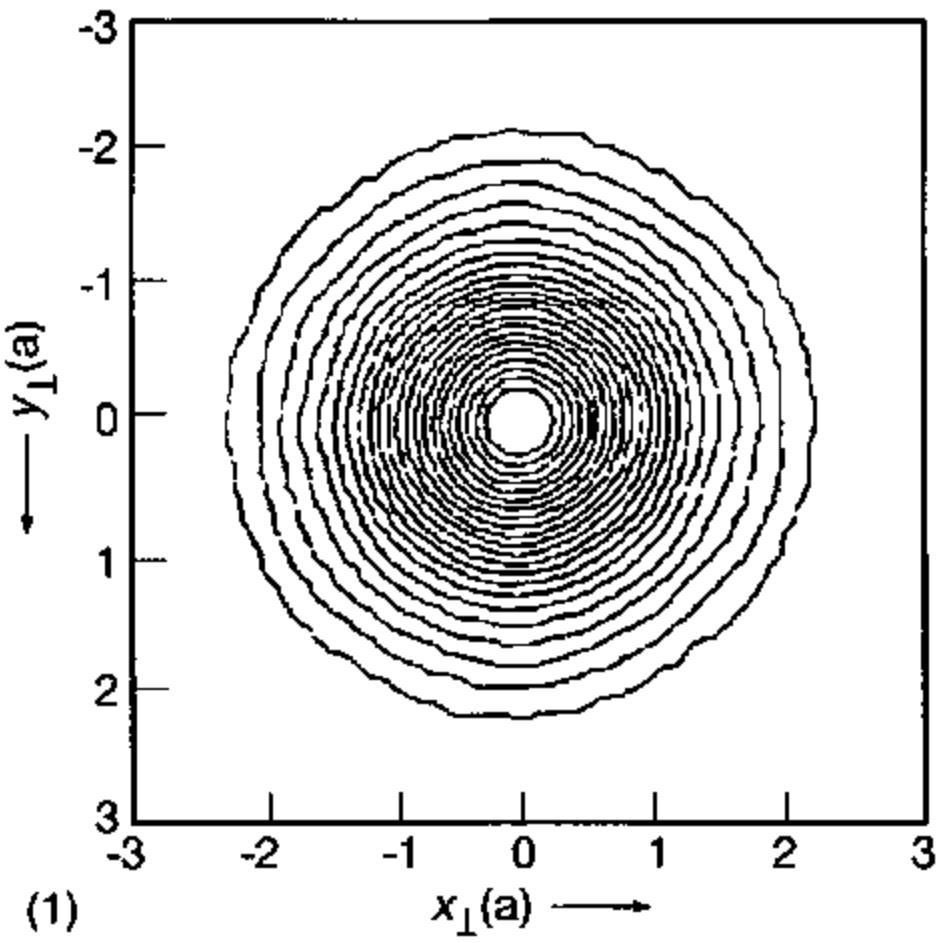
Atomic site	6D coordinates						Occupation probability		
	x_1	x_2	x_3	x_4	x_5	x_6	Al	Li	Cu
Vertex	0	0	0	0	0	0	0.56	0.02	0.42
Edge center	1/2	0	0	0	0	0	0.73	0.04	0.23
Body diagonal	$1/\tau^2$	$1/\tau^2$	0	0	0	$1/\tau^2$	0.44	0.56	0.00

In principle the shape of a multi-dimensional atoms should be a polyhedron in pseudo space, the symmetry of which is consistent with the symmetry of the quasicrystal. For simplicity the polyhedron is replaced by a sphere. In order to obtain a standard 3D Penrose tiling the 6D lattice nodes should be a unit triacontahedron. Hence the volume of the sphere should be assigned equal to that of the unit triacontahedron. However, it was found that for icosahedral quasicrystal T2—Al_6CuLi_3, a smaller sphere gives a better fit between the calculated and experimental electron diffraction pattern (Pan, Cheng and Li, 1990). In the present case a sphere with radius $R = 5.146$ Å was used accordingly. The window function is then

$$W(\mathbf{r}_\perp) = \begin{cases} 1, & |\mathbf{r}_\perp| \leq R \\ 0, & \text{otherwise} \end{cases}. \tag{17}$$

4. Test and results

A set of theoretical 6D structure factors $F(\hat{\mathbf{H}})$ was calculated according to the model given in the previous section. A spherical window function with radius equal to 5.146 Å was used to convert these structure factors to a set of $|F_q(\mathbf{H}_\parallel)|$. All the $|F_q(\mathbf{H}_\perp)|$'s less than 1% of $|F_q(000)|$ were rejected leaving in total 114 independent reflections. Finally, Gaussian distribution random errors were introduced into the $|F_q(\mathbf{H}_\parallel)|$'s making the mean error equal to



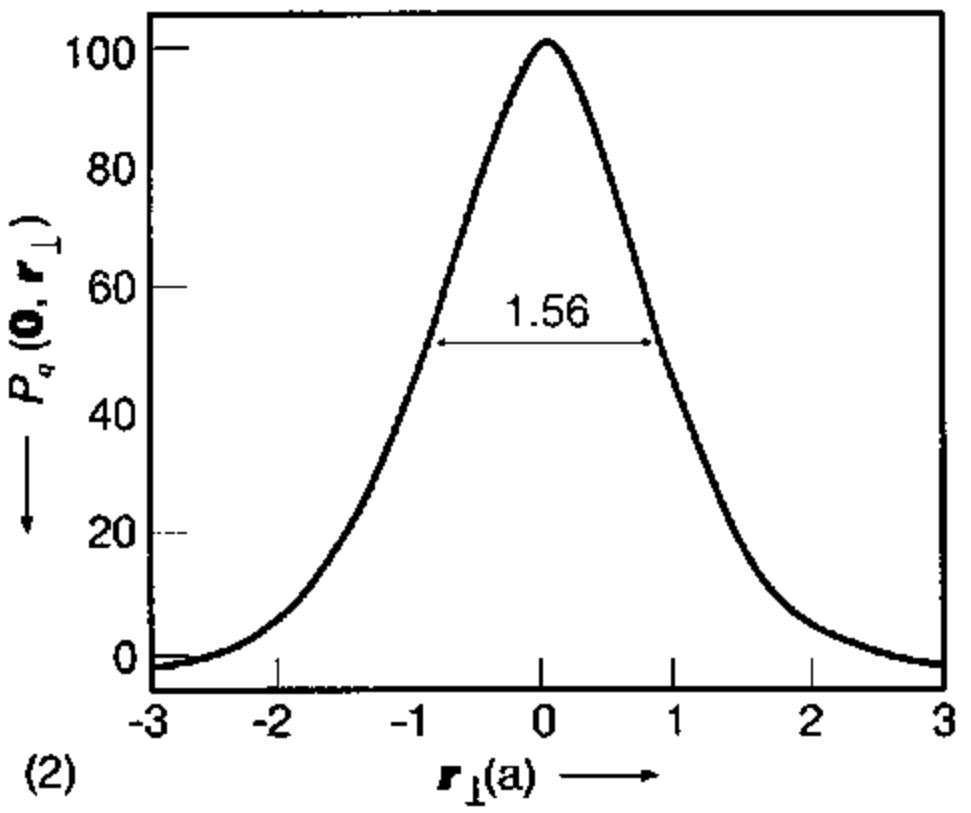


Fig. 3. Origin peak of $P_q(\mathbf{0},\mathbf{r}_\perp)$. (1) Density contour of cross section $(\mathbf{0},x_\perp,y_\perp,0)$. (2) $P_\perp(\mathbf{0},|\mathbf{r}_\perp|)$.

10%. Our test was started from such a set of $|F_q(\mathbf{H}_\parallel)|$'s to solve the quasicrystal structure.

The 'diffraction data' $|F_q(\mathbf{H}_\parallel)|$ were first converted to $|F_q(\hat{\mathbf{H}})|$ by indexing them in 6D space. The Patterson function $FT^{-1}[|F_q(\hat{\mathbf{H}})|^2]$ was then calculated from these 114 independent reflections and the width at half height of its origin peak (Fig. 3) was measured to determine the window function (Xiang, Li and Fan, 1990). The radius of the projection window so obtained is 0.78a, which is approximately equal to 5.57 Å (0.42 Å greater than the true radius). This value was used to convert $|F_q(\hat{\mathbf{H}})|$ into a set of 6D structure-factor magnitudes $|F(\hat{\mathbf{H}})|$. E values in 6D space were obtained from $|F(\hat{\mathbf{H}})|$ in a way similar to that used in 3D space. Direct-method

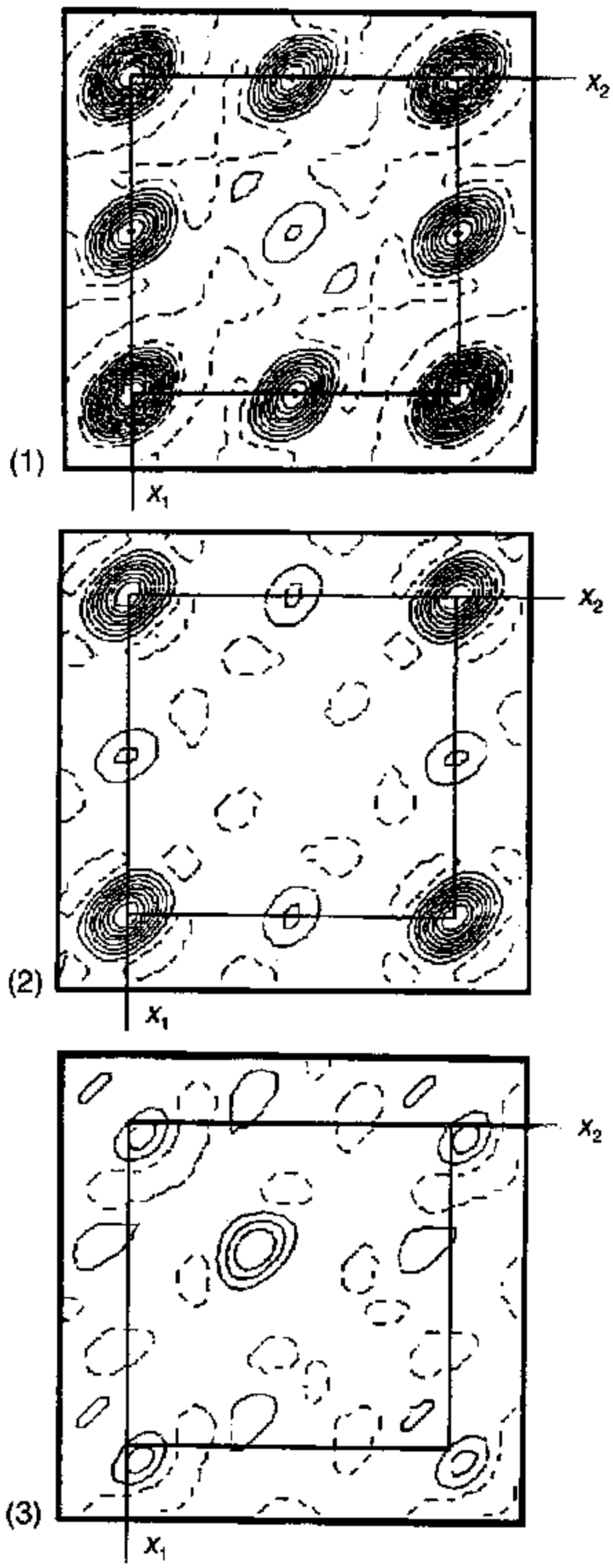


Fig. 4. Density contour of E-map of the 6D crystal structure model obtained by using derived phases of the best set. (1) Cross section $(x_1,x_2,0,0,0,0)$. (2) Cross section $(x_1,x_2,0,0,1/2)$. (3) Cross section $(x_1,x_2,0,0,0,1/\tau^2)$.

phasing by the random starting tangent refinement procedure (Yao, 1981) was performed for the 114 independent reflections. 100 trial sets were calculated. The top 9 sets with the highest combined figures of merit led to

a 6D E-map showing all the atoms of the theoretical model with both correct positions and appropriate heights (Fig. 4).

Since the radius of the window function has great influence on the resulting values of $|F(\hat{\mathbf{H}})|$. An additional test was done using a radius with even larger error. The value used is 5.72 Å, which is 10% and 0.57 Å larger than the true value. In this case the direct method still led to an E-map showing the complete structure[1].

5. Discussion

By converting the diffraction intensities of a quasicrystal to a set of structure-factor magnitudes of a 6D regular periodic structure, we can get rid of the nonperiodicity of the quasicrystal and make use of the existent methods to solve the structure. The determination of the window function is the most important step for the conversion. However the accuracy of the parametes describing the window function is not as important as expected. It was proved that direct methods can tolerate great errors in the parameters of the window function. Hence in the case that the window function has a shape different greatly from that of a sphere and/or that the window function is not the same for different atoms, it is still possible, as a first approximation, to use an overall window function with spherical shape. More accurate window-function parameters can be obtained after the structure has been roughly solved.

Among the 114 independent reflections used in the test, over ninety ones have intensity $I_q(\hat{\mathbf{H}}) > 0.001 \cdot I_{\max}$ ($I_{\max}$ is the greatest intensity except the $I_q(0,0,0,0,0,0)$). Although the used set of independent reflections is slightly bigger than that can be obtained from experiment, it is reasonable for testing a new procedure. To decrease the starting reflections will lead to a larger error in the determination of projection window. When the measured radius of projection window is too rough for direct method to tolerate, a certain refinement as suggested by Xiang, Li and Fan (1990) can be done.

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[1] A list of the phases can be ordered referring to the no. CSD 55771, names of the authors and citation of the paper at the Fachinformationszentrum Karlsruhe, Gesellschaft für wissenschaftlich-technische Information mbH, D-7514 Eggenstein-Leopoldshafen 2, Germany.

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Appendix

Let E^6 denote the 6D space in which the 6D hypercubic lattice is defined, and

$$E^6 = E_{\parallel} \bigoplus E_{\perp}, \tag{A1}$$

where $E_{\perp}$ denote the 3D subspace complementary to the subspace $E_{\parallel}$ of E^6 and is named pseudo space.

When the Cartesian coordinate system is adopted to both $E_{\parallel}$ and $E_{\perp}$, with the three orthogonal 2-fold symmetric axes of the icosahedron as the basis coordinate vectors $\mathbf{a}_{\parallel x}, \mathbf{a}_{\parallel y}, \mathbf{a}_{\parallel z}$ and $\mathbf{a}_{\perp x}, \mathbf{a}_{\perp y}, \mathbf{a}_{\perp z}$, the orientation of $E_{\parallel}$ relative to the lattice is determined by

$$\begin{pmatrix} \mathbf{a}_{\parallel x} \\ \mathbf{a}_{\parallel y} \\ \mathbf{a}_{\parallel z} \\ \mathbf{a}_{\perp x} \\ \mathbf{a}_{\perp y} \\ \mathbf{a}_{\perp z} \end{pmatrix} = \bar{\mathbf{T}} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \mathbf{a}_4 \\ \mathbf{a}_5 \\ \mathbf{a}_6 \end{pmatrix} \tag{A2}$$

where

$$T = 1/\sqrt{2\tau+4} \begin{pmatrix} \tau & 0 & 1 & -1 & 0 & \tau \\ \tau & 0 & -1 & -1 & 0 & -\tau \\ 0 & 1 & -\tau & 0 & \tau & 1 \\ -1 & \tau & 0 & -\tau & -1 & 0 \\ 0 & 1 & \tau & 0 & \tau & -1 \\ 1 & \tau & 0 & \tau & -1 & 0 \end{pmatrix} \tag{A3}$$

is a transformation matrix satisfying $T\tilde{T} = \tilde{T}T = I$ (I is a 6×6 unit matrix, $\sim$ denotes the transpositional operator), $\tau = (1+\sqrt{5})/2$. Then

$$\hat{\mathbf{r}} = \sum_{i=1}^{6} x_i \mathbf{a}_i$$

$$= (x_1, x_2, x_3, x_4, x_5, x_6) \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \mathbf{a}_4 \\ \mathbf{a}_5 \\ \mathbf{a}_6 \end{pmatrix}$$

$$= (x_{\parallel}, y_{\parallel}, z_{\parallel}) \begin{pmatrix} \mathbf{a}_{\parallel x} \\ \mathbf{a}_{\parallel y} \\ \mathbf{a}_{\parallel z} \end{pmatrix} + (x_{\perp}, y_{\perp}, z_{\perp}) \begin{pmatrix} \mathbf{a}_{\perp x} \\ \mathbf{a}_{\perp y} \\ \mathbf{a}_{\perp z} \end{pmatrix}$$

$$= \mathbf{r}_{\parallel} + \mathbf{r}_{\perp}. \tag{A4}$$

Thus the 6D reciprocal lattice vectors

$$\hat{\mathbf{H}} = (h_1, h_2, h_3, h_4, h_5, h_6) \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \mathbf{b}_4 \\ \mathbf{b}_5 \\ \mathbf{b}_6 \end{pmatrix}$$

$$= (h_1, h_2, h_3, h_4, h_5, h_6)T \begin{pmatrix} \mathbf{a}^*_{\parallel x} \\ \mathbf{a}^*_{\parallel y} \\ \mathbf{a}^*_{\parallel z} \\ \mathbf{a}^*_{\perp x} \\ \mathbf{a}^*_{\perp y} \\ \mathbf{a}^*_{\perp z} \end{pmatrix}$$

$$= (h_{\parallel x}\mathbf{a}^*_{\parallel x} + h_{\parallel y}\mathbf{a}^*_{\parallel y} + h_{\parallel z}\mathbf{a}^*_{\parallel z}) + (h_{\perp x}\mathbf{a}^*_{\perp x} + h_{\perp y}\mathbf{a}^*_{\perp y} + h_{\perp z}\mathbf{a}^*_{\perp z})$$

$$= \mathbf{H}_{\parallel} + \mathbf{H}_{\perp}. \tag{A5}$$