all pairs of non-zero entries in each row. In practice, at the points (C) where the circuits are identified, appropriate entries are made in a matrix of coefficients of the circuit and sum equations.

```
      NN=(N*(N-1))/2
      DO(I=1,M);L=0;DO(J=1,N-1);DO(K=J+1,N);L=L+1
          IF(B(I,J).NE.0.0.AND.B(I,K).NE.0.0) THEN
            NP(I,L,1)=J;NP(I,L,2)=K
          ENDIF
      ENDDO;ENDDO;ENDDO
      N4=0                                          ! find 4-circuits
      DO(I=1,M-1);DO(J=I+1,M);DO(K=1,NN)
        IF(NP(J,K,1)=0) CYCLE
        IF(NP(I,K,1)=NP(J,K,1).AND.NP(I,K,2)=NP(J,K,2)) THEN
          N4=N4+1;N1=NP(I,K,1);N2=NP(I,K,2)
C             4-circuit in rows I,J and columns N1,N2
        ENDIF
      ENDDO;ENDDO;ENDDO                          ! found N4 4-circuits
      N6=0                                        ! find 6-circuits
      DO(I=1,M-2);DO(J=I+1,M-1);DO(KI=1,NN);DO(LI=1,NN)
      DO(K1=1,2);DO(K2=1,2)
        J1=2-K1/2;J2=2-K2/2
        IF(NP(I,KI,K1)=NP(J,LI,K2).AND.NP(I,KI,J1).NE.NP(J,LI,J2))THEN
          DO(K=J+1,M);DO(L=1,NN);DO(K3=1,2)
            J3=2-K3/2
            IF(NP(I,KI,J1)=NP(K,L,K3).AND.NP(J,LI,J2)=NP(K,L,J3)) THEN
              N6=N6+1;N1=NP(I,KI,K1);N2=NP(I,KI,J1);N3=NP(J,LI,J2)
C               6-circuit: row 1 = I  cols N1 and N2
C                          row 2 = J  cols N1 and N3
C                          row 3 = K  cols N2 and N3
            ENDIF
          ENDDO;ENDDO;ENDDO
        ENDIF
      ENDDO;ENDDO;ENDDO;ENDDO;ENDDO;ENDDO          ! found N6 6-circuits
```

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A Simple Approach to Quasicrystal Structure and Phason Defect Formulation*

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Abstract

The advantages of the cut or section method in describing quasicrystal structures and phason defects are given. The real and reciprocal quasilattice formulation is derived straightforwardly. It is shown that the linear phason strain which leads to the quasilattice distortion is equivalent to a rotation of physical space relative to the high-dimensional space. A continuous rotation of the physical space will make the quasilattice deviate from its idealized form and turn gradually into a periodic lattice. The derivation of a geometrical relationship between the icosahedral quasilattice and the corresponding b.c.c. lattice becomes simple and clear. This will be beneficial to the construction of a quasicrystal structure model by reference to the corresponding b.c.c. crystal structure.

1. Introduction

Soon after the discovery of icosahedral quasicrystals in rapidly solidified Al-Mn alloys (Shechtman, Blech, Gratias & Cahn, 1984), great attention was paid to the description of quasicrystal structure which has a long-range quasiperiodic translational order and long-range orientational order. The quasicrystal structure offers a new kind of incommensurate crystal structure. Its Fourier transform consists of a δ function as for periodic crystals but the point symmetries are incompatible with traditional crystallography. Some authors proposed a density wave description of quasicrystal structures (Kalugin, Kitaev & Levitov, 1985; Bak, 1985*a*, *b*; Levine, Lubensky, Ostlund, Ramaswamy, Steinhardt & Toner, 1985; Lubensky, Ramaswamy & Toner, 1985; Jaric, 1985; Nelson & Sachdev, 1985; Sachdev & Nelson, 1985). Others described the quasicrystal structure by a technique based on projection from a high-dimensional lattice to obtain the quasicrystalline lattice (Kramer & Neri, 1984; Kalugin, Kitaev & Levitov, 1985; Duneau & Katz, 1985; Elser, 1985, 1986). It was shown that the analytical formulation of quasicrystal structures derived from the projection method is identical with the density wave description (Li & Wang, 1988). The quasicrystalline lattice can also be obtained by the generalized dual method (Socolar, Steinhardt & Levine, 1985; Levine & Steinhardt, 1986; Socolar & Steinhardt, 1986) or the multigrid method (de Brujin,

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1981). In addition, an icosahedral glass model was proposed (Stephens & Goldman, 1986), which describes icosahedral quasicrystals as densely packed atomic clusters having local icosahedral symmetry.

A decade before the discovery of quasicrystals, Penrose tiling (Penrose, 1974) was known as a geometrical structure with fivefold symmetry. It has perfect quasiperiodic long-range order and can be constructed by both projection and dual methods. The Fourier transform of a Penrose tiling or of an analog of Penrose tiling shows Bragg peaks and resembles the observed diffraction patterns of quasicrystals (Mackay, 1982). High-resolution electron microscopic images show a configuration of white dots in coincidence with Penrose tiling (Bursill & Peng, 1985; Hiraga, Hirabayashi, Inoue & Masumoto, 1985; Zhang, Ye & Kuo, 1985; Li & Liu, 1986). Penrose tiling is now accepted as an important geometrical tool for describing quasicrystal structure. If the six-dimensional (6D) space is divided into two orthogonal subspaces - the physical space or parallel space $E_\parallel$ and the pseudo space or perpendicular space $E_\perp$ - the projection of a 6D cubic lattice onto the physical space which is a superplane in the 6D space gives the typical 3D Penrose tiling consisting of prolate and oblate rhombohedra (Kramer & Neri, 1984; Kalugin, Kitaev & Levitov, 1985; Duneau & Katz, 1985; Elser, 1986). The ratio between volumes of the two kinds of rhombohedra equals the golden mean $\tau=(1+5^{1/2})/2$.

The cut or section method was first proposed by de Wolff (1974) in describing incommensurate modulated structures. It gives the same result as the projection method in describing quasicrystals so that the term 'cut and projection' is popular in literature concerning quasicrystals. However, the cut description deserves recognition from the point of view of crystallography. Apart from that, the cut method provides a common tool for describing various kinds of incommensurate structures, for instance quasicrystals, incommensurate modulated structures and so-called chimney-ladder structures which consist of two different subcells related to each other irrationally in the cell dimensions along a special direction. It shows some advantages in describing quasicrystal structures (Yamamoto & Hiraga, 1988; Ishihara & Yamamoto, 1988).

In the present paper the simplicity of quasicrystal structure formulation by the cut method is demonstrated. Special attention is paid to icosahedral quasilattices distorted by the linear phason strain and the relationship between the icosahedral quasilattice and the corresponding periodic lattice.

2. Real and reciprocal quasilattice formulation

Let $L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ represent the 6D cubic lattice function which consists of a series of δ functions with their centers at the positions of lattice points

$$L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)=\sum_{\mathbf{R}_\parallel}\sum_{\mathbf{R}_\perp}\delta(\mathbf{r}_\parallel-\mathbf{R}_\parallel)\delta(\mathbf{r}_\perp-\mathbf{R}_\perp). \quad (2\text{-}1)$$

Here $\mathbf{r}_\parallel(x_\parallel, y_\parallel, z_\parallel)$ and $\mathbf{r}_\perp(x_\perp, y_\perp, z_\perp)$ denote coordinate vectors and $\mathbf{R}_\parallel$ and $\mathbf{R}_\perp$ denote lattice vectors in physical and pseudo spaces respectively. Axes $x_\parallel$, $y_\parallel$, $z_\parallel$, $x_\perp$, $y_\perp$ and $z_\perp$ are orthogonal to one another, but they are generally not parallel to the basic vectors of the 6D cubic unit cell. When all lattice nodes have a definite size and shape described by the window function $S(\mathbf{r}_\perp)$ and

$$S(\mathbf{r}_\perp)=\begin{cases}1 & \text{inside a certain region in the pseudo space}\\ 0 & \text{elsewhere,}\end{cases} \quad (2\text{-}2)$$

the lattice function becomes the convolution of $L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ with $S(\mathbf{r}_\perp)$:

$$L(\mathbf{r}_\parallel, \mathbf{r}_\perp)=S(\mathbf{r}_\perp) * L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp), \quad (2\text{-}3)$$

where $*$ denotes the operation of convolution. The corresponding reciprocal lattice is written as

$$l(\mathbf{g}_\parallel, \mathbf{g}_\perp)=s(\mathbf{g}_\perp)l_0(\mathbf{g}_\parallel, \mathbf{g}_\perp), \quad (2\text{-}4)$$

where $s(\mathbf{g}_\perp)$ and $l_0(\mathbf{g}_\parallel, \mathbf{g}_\perp)$ are the Fourier transforms of $S(\mathbf{r}_\perp)$ and $L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ respectively. Obviously, the real and reciprocal lattices are quite different in the shape of their lattice nodes and in their boundary conditions. The real lattice is unlimited. Its lattice nodes have definite size and shape along the pseudo space, but they are sharp along the physical space. The reciprocal lattice is limited and its lattice nodes are sharp along both subspaces. The section of 6D cubic lattice in the real space with the 3D physical space gives the 3D quasilattice $u(\mathbf{r}_\parallel)$. When the 6D lattice nodes have the shape of a triacontahedron, the quasilattice is a standard 3D Penrose tiling. Because the Fourier transform of a section of any function equals the projection of the Fourier transform of this function along the direction perpendicular to the sectional plane, it is easy to write down the Fourier transform of the quasilattice function as follows:

$$\begin{aligned}V(\mathbf{g}_\parallel)&=\int l(\mathbf{g}_\parallel, \mathbf{g}_\perp)\,\mathrm{d}\mathbf{g}_\perp^3\\ &=\sum_{\mathbf{G}_\parallel}\sum_{\mathbf{G}_\perp}s(\mathbf{G}_\perp)\delta(\mathbf{g}_\parallel-\mathbf{G}_\perp),\end{aligned} \quad (2\text{-}5)$$

where $\mathbf{G}_\parallel$ and $\mathbf{G}_\perp$ are the components of 6D reciprocal-lattice vectors in the physical and pseudo spaces respectively. The inverse Fourier transform of $V(\mathbf{g}_\parallel)$ gives the formula for quasilattices identical to the density wave expression:

$$u(\mathbf{r}_\parallel)=\sum_{\mathbf{G}_\parallel}\sum_{\mathbf{G}_\perp}s(\mathbf{G}_\perp)\exp(2\pi i\mathbf{r}_\parallel\mathbf{G}_\parallel). \quad (2\text{-}6)$$

Formulae (2-5) and (2-6) are the same as those obtained by the other methods. The principle and

procedure for deriving these formulae by the cut method are shown schematically in Fig. 1.

3. Structure factor of quasicrystals

Although so far the proposed quasicrystal structure models are based on distributing atoms in the physical space directly (Elser & Henley, 1985; Audier & Guyot, 1986; Henley & Elser, 1986; Audier, Sainfort & Dubost, 1986; Yang, 1988, 1989), the atomic structure of quasicrystals can also be obtained by cutting a 6D periodic structure if hyperatoms are distributed in the 6D unit cell (Li, Wang & Fan, 1987). The 6D crystal structure $\rho_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ can be written as the convolution of the lattice function $L(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ with the function $\varphi_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ which describes the atomic distribution inside the 6D unit cell:

$$\rho_0(\mathbf{r}_\parallel, \mathbf{r}_\perp) = S(\mathbf{r}_\perp) * L_0(\mathbf{r}_\parallel, \mathbf{r}_\perp) * \varphi_0(\mathbf{r}_\parallel, \mathbf{r}_\perp). \quad (3\text{-}1)$$

As far as the structure analysis by diffraction methods is concerned, $\varphi_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ and $\rho_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ are electron density functions for X-rays and are potential distribution functions for electrons. The function $S(\mathbf{r}_\perp)$ describes the shape of lattice nodes and the shape of hyperatoms in the pseudo space. The intersection of any hyperatom with the physical space gives the real atom. The expression for the 3D quasicrystal structure $\rho(\mathbf{r}_\parallel)$, which is the intersection of $\rho_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ with the physical space, can be obtained by the procedure shown in Fig. 1, namely, firstly by doing the Fourier transform of $\rho_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)$, secondly by projecting the product along the pseudo space and finally by performing the inverse Fourier transform.

$$\rho(\mathbf{r}_\parallel) = \sum_{\mathbf{G}_\parallel} \sum_{\mathbf{G}_\perp} s(\mathbf{G}_\perp) F_0(\mathbf{G}_\parallel, \mathbf{G}_\perp) \exp(2\pi i \mathbf{r}_\parallel \mathbf{G}_\parallel), \quad (3\text{-}2)$$

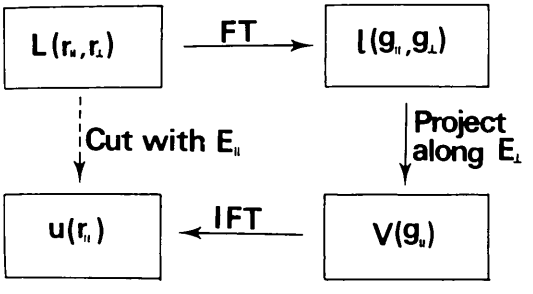

Fig. 1. Schematic diagram showing the principle of deriving the quasiperiodic lattice function in the cut description. $L(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ denotes an unlimited 6D periodic real lattice with lattice points of definite size and shape, $I(g_\parallel, g_\perp)$ denotes the 6D periodic reciprocal lattice which is limited in the pseudo space and has sharp lattice points. The projection of $I(g_\parallel, g_\perp)$ in pseudo space gives a 3D reciprocal quasilattice $V(g_\parallel)$ which has sharp lattice points and spreads along the physical space unlimitedly. The inverse Fourier transform of $V(g_\parallel)$ gives the quasiperiodic lattice $u(\mathbf{r}_\parallel)$ which is also unlimited and has sharp lattice points. $u(\mathbf{r}_\parallel)$ is none other than a section of the 6D lattice function $L(\mathbf{r}_\parallel, \mathbf{r}_\perp)$ in the physical space.

where $F_0(\mathbf{g}_\parallel, \mathbf{g}_\perp) = \mathscr{F}[\varphi_0(\mathbf{r}_\parallel, \mathbf{r}_\perp)]$ is the structure factor of the 6D crystal, $\mathscr{F}$ denotes the operation of Fourier transform. The quasicrystal structure factor is

$$F(\mathbf{G}_\parallel, \mathbf{G}_\perp) = s(\mathbf{G}_\perp) F_0(\mathbf{G}_\parallel, \mathbf{G}_\perp). \quad (3\text{-}3)$$

Here both $\mathbf{G}_\parallel$ and $\mathbf{G}_\perp$ are labeled with six icosahedral indices (Elser, 1985) or six orthogonal indices (Cahn, Shechtman & Gratias, 1986; Li & Wang, 1988) when the 6D lattice is cut irrationally by the physical space. Hence, there is a one-to-one correspondence between the structure factor of quasicrystals and the structure factor of the related high-dimensional crystal. The structure factor of the quasicrystal equals the structure factor of the corresponding high-dimensional crystal modulated by the function $s(\mathbf{G}_\perp)$.

Formula (3-3) is very useful for developing the direct method in quasicrystal structure determination (Li, Wang & Fan, 1987; Xiang, Li & Fan, 1990) by X-ray or electron-diffraction analysis and useful also for determining quasicrystal structures by use of the trial-and-error method, where the proposed structure model is given first in the 6D space.

4. Quasilattices with phason defect

The defect in the quasicrystals can be described as the phase change in the density wave expression (Lubensky, Socolar, Steinhardt, Bancel & Heiney, 1986):

$$\rho(\mathbf{r}_\parallel) = \sum_{\mathbf{G}_\parallel} \sum_{\mathbf{G}_\perp} s(\mathbf{G}_\perp) \exp[2\pi i(\mathbf{G}_\parallel \mathbf{r}_\parallel + \Delta\mathbf{G})], \quad (4\text{-}1)$$

$$\Delta\mathbf{G} = \mathbf{G}_\parallel \mathbf{u} + \mathbf{G}_\perp \mathbf{w}, \quad (4\text{-}2)$$

$\mathbf{u}$ and $\mathbf{w}$ are components of a 6D displacement vector in the physical and pseudo spaces, or the so-called phonon and phason strains respectively. The phason defect caused by the phason strain is peculiar to quasicrystals. In this section the discussion will concern only the linear phason strain. Let $\mathbf{u} = 0$ and

$$\mathbf{w} = \mathbf{M}\mathbf{r}_\parallel, \quad (4\text{-}3)$$

where $\mathbf{M}$ is a second-rank tensor, or

$$\mathbf{M} = \mathbf{e}_\perp M \mathbf{e}_\parallel, \quad (4\text{-}4)$$

$\mathbf{e}_\perp$ and $\mathbf{e}_\parallel$ denote unit vectors in the pseudo and physical spaces respectively, M is a matrix of order three and will be called the phason matrix.

Equations (4-3) and (4-4) imply that to introduce a linear phason strain into the 6D lattice makes all lattice points which have a definite shape and size in the pseudo space and are sharp in the physical space shift along the pseudo space. The shift is proportional to the phason matrix and the component of the lattice vector in the physical space. Hence, the 6D lattice and also the 3D quasilattice obtained by cutting the 6D lattice with the physical space will be distorted. In principle, the formulation of such a distorted

quasilattice, called a phason defected quasilattice, should be derived on the basis of the distorted 6D lattice. However, we are not interested in the 6D lattice itself, but only interested in its section with the physical space. In the following it will be demonstrated that introducing a linear phason strain into quasilattices is equivalent to a rotation of the physical space relative to the high-dimensional space so that the phason defected quasilattice can also be obtained by cutting the undistorted 6D lattice with a new 3D superplane.

Fig. 2 shows a two-dimensional (2D) square lattice with basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ of the same length a. All lattice nodes elongate along axis $x_\perp$ (pseudo space) to form lattice bars. The one-dimensional (1D) quasilattice is obtained by cutting the 2D lattice with axis $x_\parallel$ (physical space) which is perpendicular to axis $x_\perp$ and irrationally oriented to the 2D lattice. The 1D quasilattice obtained consists of two elemental segments of length $l = a\cos\theta$ and $s = a\sin\theta$. When $\operatorname{arccot}\theta = \tau$ and the length of the lattice bars equals $(1+s)$, the obtained 1D quasilattice is identical to the Fibonacci sequence. When a linear phason strain $w = mx_\parallel$ is introduced all lattice bars will be displaced along the direction parallel to axis $x_\perp$ by a distance $m\mathbf{R}_\parallel$; $\mathbf{R}_\parallel$ is the component of the corresponding lattice vector in the physical space. A distorted 1D quasilattice is obtained by cutting the displaced lattice bars with axis $x_\parallel$. It is none other than the 1D quasilattice obtained firstly by cutting undistorted lattice bars with an axis $x'_\parallel$ which forms an angle $\varphi = \arctan m$ with axis $x_\parallel$, and secondly by multiplying the obtained sequence by a factor $1/(1+m^2)^{1/2}$. The formulation of such a phason defected quasilattice is straightforward by setting up a new Cartesian coordinate system with axes $x'_\parallel$ and $x'_\perp$:

$$\begin{pmatrix} x'_\parallel \\ x'_\perp \end{pmatrix} = \frac{1}{1+m^2}\begin{pmatrix} 1 & -m \\ m & 1 \end{pmatrix}\begin{pmatrix} x_\parallel \\ x_\perp \end{pmatrix} = T_m \begin{pmatrix} x_\parallel \\ x_\perp \end{pmatrix}. \quad (4\text{-}5)$$

T_m is the rotation matrix describing the rotation transformation from the coordinate system $(x_\parallel, x_\perp)$ to $(x'_\parallel, x'_\perp)$.

$$\begin{pmatrix} x_\parallel \\ x_\perp \end{pmatrix} = T_m^{-1}\begin{pmatrix} x'_\parallel \\ x'_\perp \end{pmatrix} = \begin{pmatrix} 1 & m \\ -m & 1 \end{pmatrix}\begin{pmatrix} x'_\parallel \\ x'_\perp \end{pmatrix}. \quad (4\text{-}6)$$

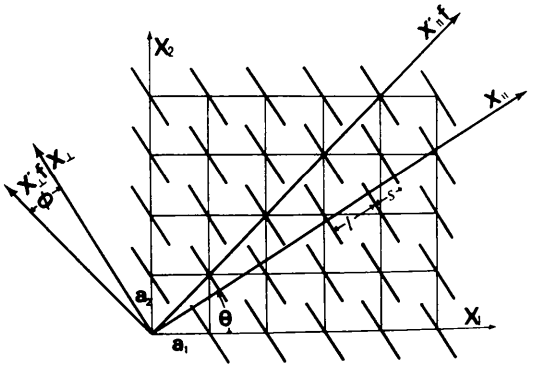

Fig. 2. Schematic diagram showing that the transformation from a 1D quasilattice to a periodic lattice is equivalent to a rotation of the physical space from axis $x_\parallel$ to $x'_\parallel$ with the help of a rotation matrix T_m. $f = (1+m^2)^{1/2}$.

Accordingly, in the reciprocal space

$$(g'_\parallel, g'_\perp) = (g_\parallel, g_\perp)\begin{pmatrix} 1 & m \\ -m & 1 \end{pmatrix}. \quad (4\text{-}7)$$

For deriving the Fourier transform of the 1D phason defected quasilattice which is the intersection of the 2D square lattice with axis $x'_\parallel$ defined by (4-5), it should be noticed that the Fourier transform of the window function remains unchanged in the new coordinate system. This is because the lattice nodes should always remain sharp in the physical space so that all lattice bars must always be considered as perpendicular to the physical space. Hence, the Fourier transform of a phason defected 1D quasilattice can be simply written as

$$V'(g'_\parallel) = \int s(g'_\perp) \sum_{\mathbf{G}'_\parallel} \sum_{\mathbf{G}'_\perp} \delta(g'_\parallel - \mathbf{G}'_\parallel)\delta(g'_\perp - \mathbf{G}'_\perp)\, dg'_\perp. \quad (4\text{-}8)$$

It should be emphasized that the new coordinated system is only a tool for formulating the phason defected quasilattice. In general, (4-5) gives only the relationship between two coordinate systems but does not give the coordinate relationship between the idealized quasilattice nodes obtained by cutting the 2D square lattice with axis $x_\parallel$ and the phason defected quasilattice nodes obtained by cutting the 2D square lattice with axis $x'_\parallel$. The only exception is the case when axis $x'_\parallel$ intercepts lattice bars at their center so that the 1D quasilattice turns into a periodic lattice. However, (4-7) always gives the right coordinate relationship between the reciprocal-lattice nodes of the idealized and the phason defected quasilattice. This is because all lattice nodes are sharp in the 2D reciprocal space and the reciprocal quasilattice nodes are projections of the sharp 2D lattice nodes. Thus the reciprocal quasilattice vectors of the phason defected quasilattice are expressed as

$$\mathbf{G}'_\parallel = \mathbf{G}_\parallel - m\mathbf{G}_\perp. \quad (4\text{-}9)$$

To illustrate clearly the change of Fourier spectra of the phason defected quasilattice, a coordinate transformation is made so that

$$V'(g_\parallel) = \int s(g_\perp) \sum_{\mathbf{G}_\parallel} \sum_{\mathbf{G}_\perp} \delta[g_\parallel - (\mathbf{G}_\parallel - m\mathbf{G}_\perp)] \times \delta[g_\perp - (\mathbf{G}_\perp + m\mathbf{G}_\parallel)]\, dg_\perp, \quad (4\text{-}10)$$

or

$$V'(g_\parallel) = s(\mathbf{G}_\perp) \sum_{\mathbf{G}_\parallel} \sum_{\mathbf{G}_\perp} \delta[g_\parallel - (\mathbf{G}_\parallel - m\mathbf{G}_\perp)], \quad (4\text{-}11)$$

here the function $s(\mathbf{G}_\perp + m\mathbf{G}_\parallel)$ is replaced by $s(\mathbf{G}_\perp)$

owing to the above reason that in the real space all lattice bars are always perpendicular to the physical space. The density wave expression of the phason defected 1D quasilattice is

$$u'(x_\parallel)=\sum_{\mathbf{G}_\parallel}\sum_{\mathbf{G}_\perp} s(\mathbf{G}_\perp)\exp\left[2\pi i x_\parallel(\mathbf{G}_\parallel-m\mathbf{G}_\perp)\right]. \quad (4\text{-}12)$$

In the case of a 3D quasilattice with a phason defect the new 6D orthogonal coordinate system $(\mathbf{r}'_\parallel, \mathbf{r}'_\perp)$ is related to the old one by

$$\begin{pmatrix}\mathbf{r}'_\parallel\\ \mathbf{r}'_\perp\end{pmatrix}=\frac{1}{k}\begin{pmatrix}I & -\mathbf{M}\\ \mathbf{M} & I\end{pmatrix}\begin{pmatrix}\mathbf{r}_\parallel\\ \mathbf{r}_\perp\end{pmatrix}=T_m\begin{pmatrix}\mathbf{r}_\parallel\\ \mathbf{r}_\perp\end{pmatrix}, \quad (4\text{-}5')$$

and

$$\begin{pmatrix}\mathbf{r}_\parallel\\ \mathbf{r}_\perp\end{pmatrix}=T_m^{-1}\begin{pmatrix}\mathbf{r}'_\parallel\\ \mathbf{r}'_\perp\end{pmatrix}=\begin{pmatrix}I & \tilde{\mathbf{M}}\\ -\tilde{\mathbf{M}} & I\end{pmatrix}\begin{pmatrix}\mathbf{r}'_\parallel\\ \mathbf{r}'_\perp\end{pmatrix}, \quad (4\text{-}6')$$

where I is the unit matrix of order 3, $\mathbf{M}$ the phason matrix, $\tilde{\mathbf{M}}$ the transpose matrix of $\mathbf{M}$ and k the multiplying factor depending on the elements of $\mathbf{M}$. In the reciprocal space

$$(g'_\parallel, g'_\perp)=(g_\parallel, g_\perp)\begin{pmatrix}I & \tilde{\mathbf{M}}\\ -\tilde{\mathbf{M}} & I\end{pmatrix} \quad (4\text{-}7')$$

and

$$\mathbf{G}'_\parallel=\mathbf{G}_\parallel-\mathbf{G}_\perp\tilde{\mathbf{M}}. \quad (4\text{-}9')$$

The Fourier transform of the 3D quasilattice with a linear phason defect is

$$V'(g_\parallel)=s(\mathbf{G}_\perp)\sum_{\mathbf{G}_\parallel}\sum_{\mathbf{G}_\perp}\delta[g_\parallel-(\mathbf{G}_\parallel-\mathbf{G}_\perp\tilde{\mathbf{M}})]. \quad (4\text{-}11')$$

The corresponding density wave expression is

$$u'(\mathbf{r}_\parallel)=\sum_{\mathbf{G}_\parallel}\sum_{\mathbf{G}_\perp} s(\mathbf{G}_\perp)\exp\left[2\pi i\mathbf{r}_\parallel(\mathbf{G}_\parallel-\mathbf{G}_\perp\tilde{\mathbf{M}})\right]. \quad (4\text{-}12')$$

The phase change caused by the phason strain is

$$\Delta\mathbf{G}=-\mathbf{G}_\perp\tilde{\mathbf{M}}. \quad (4\text{-}13)$$

According to (2-5) the diffraction intensity of quasicrystals is modulated by $|s(\mathbf{G}_\perp)|^2$ so that strong diffraction peaks generally correspond to small $\mathbf{G}_\perp$ and *vice versa*. Formula (4-13) indicates that the shift of diffraction peaks is proportional to the absolute value of $\mathbf{G}_\perp$. Hence, a weak diffraction peak is bound to have a large shift while a strong peak has a small shift, as was pointed out by Lubensky *et al.* (1986). This has been confirmed by experimental results. One more point worth noticing is that the diffraction peaks move along the direction opposite to $\mathbf{G}_\perp\tilde{\mathbf{M}}$.

Although the results obtained in this section are principally the same as those obtained by the projection method where the action of a linear phason strain is treated as the rotation of the projection strip (Cheng & Li, 1990), here the derivation is much simplified.

5. From icosahedral lattice to b.c.c. lattice

Recently, the intermediate states between the I and b.c.c. phases were first revealed clearly in Al-Cu-Mg alloy by electron diffraction and high-resolution electron microscopy (Li, Teng, Huang, Chen & Chen, 1988). Later, a similar phenomenon was observed by the X-ray precession technique (Mai, Zhang, Hui, Huang & Chen, 1988). Furthermore, a series of electron-diffraction patterns showing an almost continuous transformation from the I to the b.c.c. phase was obtained in Al-Cu-Li alloy (Li, Pan, Tao, Hui, Mai, Chen & Cai, 1989). All of these imply a close relationship between the I and b.c.c. phases. Mai, Tao, Zeng & Zhang (1988) have given an illustration of this. However, some points need clarifying. This section aims to derive the relationship between the I phase and the b.c.c. phase more strictly but rather simply by the cut method.

The 6D cubic lattice is described by a 6D orthogonal coordinate system $(x_1, x_2, x_3, x_4, x_5, x_6)$ with six basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5$ and $\mathbf{a}_6$ which form a 6D unit cell of edge length a. If the 6D space is divided into two orthogonal subspaces - the physical space $E_\parallel$ and the pseudo space $E_\perp$, the components of the six basis vectors in $E_\parallel$ are six basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4, \mathbf{e}_5$ and $\mathbf{e}_6$ in the icosahedral coordinate system (Elser, 1986; Katz & Duneau, 1986) which is widely used in describing icosahedral quasicrystals. Another set of six basis vectors in the 6D space can be selected such that three vectors, for instance, $\mathbf{a}_{\parallel x}$, $\mathbf{a}_{\parallel y}$ and $\mathbf{a}_{\parallel z}$ are in the physical space, while the other three, $\mathbf{a}_{\perp x}$, $\mathbf{a}_{\perp y}$ and $\mathbf{a}_{\perp z}$ are in the pseudo space. The transformation from $\mathbf{a}_{\parallel x}, \mathbf{a}_{\parallel y}, \mathbf{a}_{\parallel z}, \mathbf{a}_{\perp x}, \mathbf{a}_{\perp y}, \mathbf{a}_{\perp z}$ to $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6$ is performed by a matrix T:

$$(\mathbf{a}_{\parallel x}, \mathbf{a}_{\parallel y}, \mathbf{a}_{\parallel z}, \mathbf{a}_{\perp x}, \mathbf{a}_{\perp y}, \mathbf{a}_{\perp z})=(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6)T. \quad (5\text{-}1)$$

The transformation matrix T was given by Cahn *et al.* (1986) and by Li & Wang (1988). However, the right choice of the relative configuration between two sets of basis vectors is essential for obtaining a convenient form of the phason matrix to describe the transformation from icosahedral quasicrystals to b.c.c. crystals. If axes $x_\parallel, y_\parallel, z_\parallel$ and axes $x_\perp, y_\perp, z_\perp$ are arranged relative to the corresponding icosahedral basis vectors as shown in Fig. 3, matrix T will have the form

$$T=\frac{1}{(2+2\tau^2)^{1/2}}\begin{pmatrix}\tau & 0 & 1 & -1 & 0 & \tau\\ \tau & 0 & -1 & -1 & 0 & -\tau\\ 0 & 1 & -\tau & 0 & \tau & 1\\ -1 & \tau & 0 & -\tau & -1 & 0\\ 0 & 1 & \tau & 0 & \tau & -1\\ 1 & \tau & 0 & \tau & -1 & 0\end{pmatrix}. \quad (5\text{-}2)$$

According to (5-2), vectors $\mathbf{a}_{\parallel x}$, $\mathbf{a}_{\parallel y}$, $\mathbf{a}_{\parallel z}$, $\mathbf{a}_{\perp x}$, $\mathbf{a}_{\perp y}$ and $\mathbf{a}_{\perp z}$ are the same length as vectors $\mathbf{a}_j$ $(j=1,2,\ldots,6)$ and $\mathbf{a}_{\parallel x}$, $\mathbf{a}_{\parallel y}$, $\mathbf{a}_{\parallel z}$ and $\mathbf{a}_{\perp x}$, $\mathbf{a}_{\perp y}$, $\mathbf{a}_{\perp z}$ are parallel to three twofold axes of the basis icosahedron in the physical and pseudo spaces respectively.

In the following it will be proved that a peculiar linear phason strain with the phason matrix

$$\mathbf{M}=\begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{pmatrix} \tag{5-3}$$

makes the icosahedral quasilattice distort in such a way that the lattice takes a form in between quasiperiodic and periodic states or turns into the b.c.c. lattice when m takes a definite value.

The 6D space can also be divided into another pair of subspaces $E'_{\parallel}$ and $E'_{\perp}$ with basis vectors $\mathbf{a}'_{\parallel x}$, $\mathbf{a}'_{\parallel y}$, $\mathbf{a}'_{\parallel z}$ and $\mathbf{a}'_{\perp x}$, $\mathbf{a}'_{\perp y}$, $\mathbf{a}'_{\perp z}$ respectively. The transformation from $E_{\parallel}$ and $E_{\perp}$ to $E'_{\parallel}$ and $E'_{\perp}$ is performed by the matrix

$$T_m^{-1}=\begin{pmatrix} I & -M \\ M & I \end{pmatrix} \tag{5-4}$$

and

$$(\mathbf{a}'_{\parallel x}, \mathbf{a}'_{\parallel y}, \mathbf{a}'_{\parallel z}, \mathbf{a}'_{\perp x}, \mathbf{a}'_{\perp y}, \mathbf{a}'_{\perp z}) = (\mathbf{a}_{\parallel x}, \mathbf{a}_{\parallel y}, \mathbf{a}_{\parallel z}, \mathbf{a}_{\perp x}, \mathbf{a}_{\perp y}, \mathbf{a}_{\perp z})T_m^{-1}. \tag{5-5}$$

The intersection of the 6D hypercubic lattice with $E'_{\parallel}$ gives the 3D quasilattice distorted by the linear phason strain. The transformation from $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6)$ to $(\mathbf{a}'_{\parallel x}, \mathbf{a}'_{\parallel y}, \mathbf{a}'_{\parallel z}, \mathbf{a}'_{\perp x}, \mathbf{a}'_{\perp y}, \mathbf{a}'_{\perp z})$ is performed by the product matrix $T_m^{-1}T$:

$$(\mathbf{a}'_{\parallel x}, \mathbf{a}'_{\parallel y}, \mathbf{a}'_{\parallel z}, \mathbf{a}'_{\perp x}, \mathbf{a}'_{\perp y}, \mathbf{a}'_{\perp z}) = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6)TT_m^{-1} \tag{5-6}$$

$$TT_m^{-1}=\frac{1}{(2+2\tau^2)^{1/2}}\begin{pmatrix} t_1 & 0 & t_2 & -t_2 & 0 & t_1 \\ t_1 & 0 & -t_2 & -t_2 & 0 & -t_1 \\ 0 & t_2 & -t_1 & 0 & t_1 & t_2 \\ -t_2 & t_1 & 0 & -t_1 & -t_2 & 0 \\ 0 & t_2 & t_1 & 0 & t_1 & -t_2 \\ t_2 & t_1 & 0 & t_1 & -t_2 & 0 \end{pmatrix}, \tag{5-7}$$

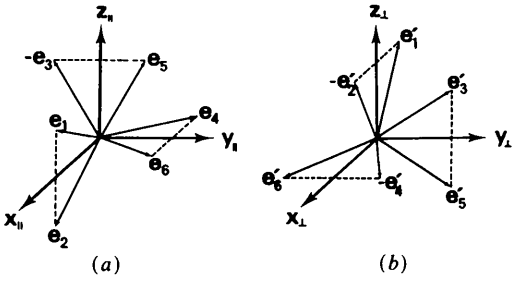

Fig. 3. Relationship between the icosahedral coordinate system and the orthogonal coordinate system in (a) physical and (b) pseudo spaces.

where $t_1=\tau+m$ and $t_2=1-m\tau$. When $m=0$, *i.e.* when the phason strain vanishes, the product matrix degenerates to matrix T so that the intersection of the 6D hypercubic lattice with the subspace $E'_{\parallel}$ gives a perfect or an idealized icosahedral quasilattice. When t_1/t_2 becomes a ratio of two integers, the section would be a 3D periodic lattice. When $t_1/t_2=1$ or $m=-(\tau-1)/(\tau+1)=-0{\cdot}236$,

$$TT_m^{-1}=\frac{(2+2\tau^2)^{1/2}}{2}\begin{pmatrix} 1 & 0 & 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & -1 \\ 0 & 1 & -1 & 0 & 1 & 1 \\ -1 & 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & 0 & 1 & -1 \\ 1 & 1 & 0 & 1 & -1 & 0 \end{pmatrix}. \tag{5-8}$$

In this case the corresponding index relationship in the reciprocal space is

$$(h'_{\parallel}, k'_{\parallel}, l'_{\parallel}, h'_{\perp}, k'_{\perp}, l'_{\perp}) = (h_1, h_2, h_3, h_4, h_5, h_6)TT_m^{-1}. \tag{5-9}$$

If we let $h\equiv h'_{\parallel}$, $k\equiv k'_{\parallel}$ and $l\equiv l'_{\parallel}$, then

$$(h,k,l)=\frac{(2+2\tau^2)^{1/2}}{2}(h_1,\ldots,h_6)\begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & -1 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{5-10}$$

Equation (5-10) shows that the three reciprocal basis vectors for the physical space are still of the same length. Therefore, they form a reciprocal cubic unit cell.

In order to have integer indices h, k, l, the reciprocal-lattice parameter a_c^* should be

$$a_c^*=\frac{(2+2\tau^2)^{1/2}}{2\tau^2}a^*, \tag{5-11}$$

where $a^*=1/a$. Then the corresponding lattice parameter in the real space is

$$a_c=\frac{2\tau^2}{(2+2\tau^2)^{1/2}}a=\frac{2\tau^2}{(1+\tau^2)^{1/2}}a_R, \tag{5-12}$$

where a_R is the edge length of rhombohedra which form the 3D Penrose tiling. Let $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ represent the three basis vectors of the cubic lattice in the real space, then the relationship of $\mathbf{a}_c$, $\mathbf{b}_c$, $\mathbf{c}_c$ with the six 6D basis vectors $\mathbf{a}_1,\ldots,\mathbf{a}_6$ is obtained from (5-6), (5-8) and (5-12) as follows:

$$\begin{aligned} \mathbf{a}_c &= \tau^2(\mathbf{a}_1+\mathbf{a}_2-\mathbf{a}_4+\mathbf{a}_6)/(2+2\tau^2)^{1/2}, \\ \mathbf{b}_c &= \tau^2(\mathbf{a}_3+\mathbf{a}_4+\mathbf{a}_5+\mathbf{a}_6)/(2+2\tau^2)^{1/2}, \\ \mathbf{c}_c &= \tau^2(\mathbf{a}_1-\mathbf{a}_2-\mathbf{a}_3+\mathbf{a}_5)/(2+2\tau^2)^{1/2}. \end{aligned} \tag{5-13}$$

Obviously, the diagonal of the cubic unit cell has the length

$$|\mathbf{a}_c+\mathbf{b}_c+\mathbf{c}_c| = \tau^2|2\mathbf{a}_1-2\mathbf{a}_5+2\mathbf{a}_6|/(2+2\tau^2)^{1/2}. \quad (5\text{-}14)$$

Equation (5-14) implies that there is a lattice node at the center of the body diagonal. Hence, the cubic lattice is of the b.c.c. type.

It was determined that the edge length of rhombohedra for the icosahedral phase (I phase) in Al-Cu-Li alloy is 5·04 Å (Shen, Poon, Dmowski, Egami & Shiflet, 1987). According to (5-12) the corresponding b.c.c. lattice parameter would be 13·9 Å. This is in agreement with the lattice parameter of the b.c.c. phase R-Al_5CuLi_3 (Cherkashin, Krinyakevich & Oleksiv, 1963).

6. Discussion

The quasicrystal structure can be described by the cut method and the projection method. The cut method can be used to describe various kinds of modulated structures including the incommensurate modulated structure, the chimney-ladder structure and the quasicrystal structure. But not all kinds of modulated structure can be described by the projection method. For instance, the projection method becomes powerless against the incommensurate modulated structure.

Although the cut method gives the same results as the projection method in describing quasicrystals, the proof of the discrete character of the Fourier transform of the quasicrystal structure is straightforward and the quasicrystal structure formulation becomes simple in the cut description.

The linear phason strain which leads to a distortion of the quasilattice is equivalent to the strip rotation in the projection method, while in the cut method it is equivalent to the rotation of physical space relative to the high-dimensional space. When the physical space, starting from the irrational orientation, rotates continuously towards a rational orientation, the quasilattice turns continuously towards a periodic lattice (see also Kramer, 1987). This is confirmed experimentally by two series of electron diffraction patterns showing an almost continuous transformation from the idealized icosahedral quasicrystal in Al-Cu-Li alloy ($T2$ phase) towards the b.c.c. phase (R phase) (Li *et al.*, 1989). The geometrical relationship between the quasilattice and the phason related periodic lattice can be derived under both the projection method and the cut method. However, in the latter case the derivation becomes simple and clear.

In some alloys such as Al-Cu-Li and Al-Cu(Zn)-Mg the I phase coexists with a b.c.c. phase close in composition (Sainfort & Dubost, 1986; Henley & Elser, 1986). In such cases the lattice of the b.c.c. phase can be considered as an I phase extremely distorted by a peculiar linear phason strain (Li *et al.*, 1989). Hence, it is reasonable to construct the structure model of the I phase on the basis of the corresponding b.c.c. phase.

Elser & Henley (1985), Audier & Guyot (1986), Henley & Elser (1986), Audier *et al.* (1986) and Yang (1988, 1989) proposed icosahedral quasicrystal structure models by directly distributing atoms in the 3D space. Another possible approach to quasicrystal structure models is first to distribute hyperatoms in the 6D space and then to obtain the 3D quasicrystal structure model by cut or projection. The advantage of this approach is to give the convenience of applying the diffraction analysis technique developed for crystal structure research to the case of quasicrystals. The argument and the formulation of the transformation from the icosahedral quasilattice to the corresponding b.c.c. lattice and the experimental evidence of the existence of intermediate states between the I phase and the b.c.c. phase are beneficial to the distribution of hyperatoms in the 6D space. A 6D crystal is under construction for the Al-Cu-Li quasicrystal. The result will be published elsewhere.

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