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The connection between the reciprocal-lattice symmetries of an icosahedral quasi-crystal and those of cubic crystals

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Abstract. The connection between the reciprocal-lattice symmetries of an icosahedral quasi-crystal and those of cubic crystals is investigated using group theory and the projection method. The reciprocal lattice could be transformed from an icosahedral quasi-crystal into crystals with m3 or m3m symmetries under the action of soft-phason strain. There are several intermediate states between the icosahedral quasi-crystal and cubic crystals. The effect of the soft-phason strain is also discussed.

1. Introduction

The discovery that a rapidly cooled Al–Mn alloy has an icosahedral diffraction pattern [1] has posed an exciting crystallographic problem. This alloy has an icosahedral symmetry which is inconsistent with the usual lattice translations for periodic crystals. The diffraction spots of an icosahedral quasi-crystal do not form a regular periodic pattern and cannot be indexed by the three Miller indices *hkl*. A natural way of representing the quasi-crystal diffraction pattern is the method in which a reciprocal lattice in higher-dimension ordinary space is projected into three-dimensional (3D) hyperplane (physical space). For the icosahedral quasi-crystal (Al–Cu–Li), the higher-dimensional reciprocal lattice is a single cubic lattice in a six-dimensional space (6D) [2, 3]. The distortions of the diffraction patterns of quasi-crystals have been reported in many papers [4–6], and the phason strain is used to explain the distortions [7]. However, the question of whether the distorted quasi-crystal phase is an intermediate phase between quasi-crystals and crystals and of how they are connected together have not been resolved.

In this paper, we use group theory and the projection method to show how icosahedral symmetries of quasi-crystals could be connected with m3m or m3 symmetries of a crystal (in the reciprocal space) by the action of soft-phason strain. Moreover, not only can the quasi-crystal diffraction pattern be represented by projecting the 6D hyper-lattice into the 3D physical space, but so also can the crystal diffraction pattern. The effect of the soft-phason strain is to change the 3D hyperplane ($Z_3^{\parallel}$) in 6D space. The theoretical and experimental results agree very well.

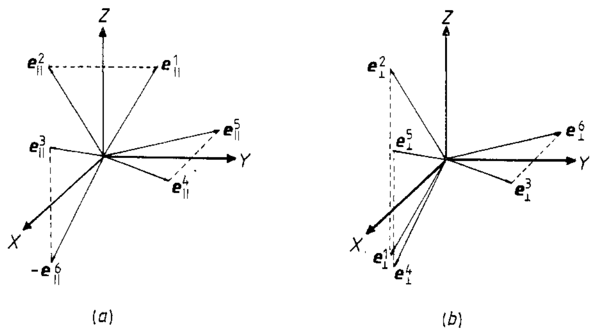

Figure 1. Geometry of the vectors in the two 3D hyperplanes (a) $Z_3^\parallel$ with vectors $e^i_\parallel$, and (b) $Z_3^\perp$ with vectors $e^i_\perp$. ($i = 1, \ldots, 6$).

Table 1. Character table of the icosahedral point group [$\tau = (1 + \sqrt{5})/2$].

I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$
Γ_1	1	1	1	1	1
Γ_3	3	τ	$1-\tau$	0	-1
$\Gamma_{3'}$	3	$1-\tau$	τ	0	-1
Γ_4	4	-1	-1	1	0
Γ_5	5	0	0	-1	1
Δ	6	1	1	0	-2

2. Theoretical analysis

According to the projection method, the basis vectors e^i of the 6D reciprocal lattice (Z_6) are projected into two 3D hyperplanes, $Z_3^\parallel$ and $Z_3^\perp$, to generate vectors $e^i_\parallel$ and $e^i_\perp$, respectively, where $e^i = (e^i_\parallel, e^i_\perp)$ ($i = 1, \ldots, 6$). To satisfy the symmetry of an Al–Cu–Li quasi-crystal which has a symmetry of $\bar{5}\bar{3}2/m$ [8], the basis vectors $e^i_\parallel$ are lined up with the six fivefold symmetry axes of an icosahedron. In the pseudo-space ($Z_3^\perp$), the set of vectors $e^i_\perp$ also forms an icosahedral set. The vectors of $e^i_\parallel$ and $e^i_\perp$ chosen are shown in figure 1. Then all the diffraction spots can be indexed by integer linear combinations of the six vectors $e^i_\parallel$. A general Bragg vector may be written as follows:

$$G_\parallel = \frac{\pi}{a}\sum_{i=1}^{6} n_i e^i_\parallel \tag{1}$$

where the n_i are integers and a is an element constant which represents the edge length of the rhombohedral cells that make up the 3D Penrose tiling [3]. For each Bragg vector given by equation (1), there corresponds a vector in the pseudo-space:

$$G_\perp = \frac{\pi}{a}\sum_{i=1}^{6} n_i e^i_\perp . \tag{2}$$

In general, the symmetry operations in the 6D space produce a 6D representation Δ of the icosahedral group I, which can be decomposed into irreducible representations of I. The character table of the icosahedral group I is shown in table 1. It is clear that

$$\Delta = \Gamma_3 + \Gamma_{3'} .$$

Therefore the 6D space can be decomposed into two 3D-invariant subspaces. In 6D space (Z_6) the six basis vectors e^i can be given by

$$e^1=\begin{bmatrix}1\\0\\0\\0\\0\\0\end{bmatrix}\qquad e^2=\begin{bmatrix}0\\1\\0\\0\\0\\0\end{bmatrix}\qquad e^3=\begin{bmatrix}0\\0\\1\\0\\0\\0\end{bmatrix}$$

$$e^4=\begin{bmatrix}0\\0\\0\\1\\0\\0\end{bmatrix}\qquad e^5=\begin{bmatrix}0\\0\\0\\0\\1\\0\end{bmatrix}\qquad e^6=\begin{bmatrix}0\\0\\0\\0\\0\\1\end{bmatrix}.$$

They are the basis vectors of the representation Δ. The linear combinations of these basis vectors, $e'^i=\sum_{i=1}^{6} a_i e^i$, consist of six new basis vectors in the 6D space, three of them, e'^1, e'^2 and e'^3, are the orthogonal basis vectors of the irreducible representation Γ_3 of group I and define a 3D-invariant subspace (physical space) while the others, e'^4, e'^5 and e'^6, are the orthogonal basis vectors of an irreducible representation $\Gamma_{3'}$ of group I and define another 3D-invariant subspace (pseudo-space). By using the method of group representation theory, the six new basis vectors e'^i are expressed in the 6D space (Z_6) by

$$e'^1=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}0\\0\\\tau\\1\\-1\\-\tau\end{bmatrix}\qquad e'^2=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}1\\-1\\0\\\tau\\\tau\\0\end{bmatrix}\qquad e'^3=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}\tau\\\tau\\1\\0\\0\\1\end{bmatrix}$$

$$e'^4=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}0\\0\\1\\-\tau\\\tau\\-1\end{bmatrix}\qquad e'^5=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}-1\\-1\\\tau\\0\\0\\\tau\end{bmatrix}\qquad e'^6=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}-\tau\\\tau\\0\\1\\1\\0\end{bmatrix}.$$

The process of projecting a vector of 6D space into the 3D hyperplane $Z_3^{\parallel}$ can be represented by the projection matrix $\mathbf{P}_\parallel$, and into the 3D space $Z_3^{\perp}$ by $\mathbf{P}_\perp$. The projection matrices $\mathbf{P}_\parallel$ and $\mathbf{P}_\perp$ are given by

$$\mathbf{P}_\parallel=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}0&0&\tau&1&-1&-\tau\\1&-1&0&\tau&\tau&0\\\tau&\tau&1&0&0&1\end{bmatrix}$$

$$\mathbf{P}_\perp=\frac{1}{\sqrt{1+\tau^2}}\begin{bmatrix}0&0&1&-\tau&\tau&-1\\-1&-1&\tau&0&0&\tau\\-\tau&\tau&0&1&1&0\end{bmatrix}.$$

Therefore, $e^i_\parallel = \mathbf{P}_\parallel e^i$ and $e^i_\perp = \mathbf{P}_\perp e^i$.

From the Landau theory, the density wave $\rho(r)$ of the L phase can be given by [9]

$$\rho(r) = \sum_{G_\parallel \in Z_3^\parallel} |\rho_G| \exp[\mathrm{i}(r \cdot G_\parallel + U(x) \cdot G_\parallel + W(x) \cdot G_\perp)]$$

where $G_\parallel \in Z_3^\parallel$ and $G_\perp \in Z_3^\perp$; $U(x)$ is the rigid-translation distortion (phonon strain), and $W(x)$ is the phase-displacement distortion (phason strain). The hydrodynamic theory for the icosahedral quasi-crystal predicts that U relaxes rapidly via phonon modes, whereas W relaxes extremely slowly.

If the spatial variations in W are approximately linear over a given small region of quasi-crystal, the phason field could be given by $W(x) = W(0) + X \cdot \mathbf{M}$, where $\mathbf{M}$ is a second-rank tensor, x is a vector transforming under the irreducible representation Γ_3 of the icosahedral group, and W under $\Gamma_{3'}$. It is evident that the effect of a linear phason strain W is to shift the Bragg peaks from the wavevector $G_\parallel$ of an unstrained quasi-crystal into that of $G_\parallel + \mathbf{M}G_\perp$ [7].

The second-rank tensor $\mathbf{M}$ can be obtained according to the symmetry of distorted quasi-crystal obtained in our experiment [10]; we have

$$\mathbf{M} = \alpha \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

where α is a parameter expressing the strength of soft-phason field.

If we project a vector

$$L = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \\ n_6 \end{bmatrix}$$

from the Z_6-space into the 3D space $Z_3^\parallel$, the vector $G_\parallel$ in the $Z_3^\parallel$-space could be written

$$G_\parallel = \frac{\pi}{a} \sum_{i=1}^{6} n_i e^i_\parallel = \frac{\pi}{a} \mathbf{P}_\parallel L = \frac{\pi}{a} \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} \tau(n_3 - n_6) + n_4 - n_5 \\ n_1 - n_2 + \tau(n_4 + n_5) \\ \tau(n_1 + n_2) + n_3 + n_6 \end{bmatrix}.$$

Similarly the partner in pseudo-space $Z_3^\perp$ is given by

$$G_\perp = \frac{\pi}{a} \sum_{i=1}^{6} n_i e^i_\perp = \frac{\pi}{a} \mathbf{P}_\perp L = \frac{\pi}{a} \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} n_3 - n_6 + \tau(n_5 - n_4) \\ -n_1 - n_2 + \tau(n_3 + n_6) \\ \tau(n_2 - n_1) + n_4 + n_5 \end{bmatrix}.$$

Then the wavevector $G'_\parallel$ which is distorted from $G_\parallel$ by the action of phason strain is

$$G'_\parallel = G_\parallel + \mathbf{M}G_\perp = \frac{\pi}{a} \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} (\tau - \alpha)(n_3 - n_6) + (1 + \alpha\tau)(n_4 - n_5) \\ (\tau - \alpha)(n_4 + n_5) + (1 + \alpha\tau)(n_1 - n_2) \\ (\tau - \alpha)(n_1 + n_2) + (1 + \alpha\tau)(n_3 + n_6) \end{bmatrix} = \frac{\pi}{a} \mathbf{P}^\alpha_\parallel L.$$

So

$$\mathbf{P}^\alpha_\parallel = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 0 & 0 & \tau - \alpha & 1 + \alpha\tau & -1 - \alpha\tau & -\tau + \alpha \\ 1 + \alpha\tau & -1 - \alpha\tau & 0 & \tau - \alpha & \tau - \alpha & 0 \\ \tau - \alpha & \tau - \alpha & 1 + \alpha\tau & 0 & 0 & 1 + \alpha\tau \end{bmatrix}.$$

Under the action of phason strain, the hyperplane $Z_3^{\parallel}$ has been transformed into another hyperplane $Z_3^{\parallel\alpha}$. The six basis vectors in Z_6 are projected into $Z_3^{\parallel\alpha}$; one can obtain

$$e_{\parallel\alpha}^1 = \mathbf{P}_{\parallel}^{\alpha} e^1 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 0 \\ 1+\alpha\tau \\ \tau-\alpha \end{bmatrix} \qquad e_{\parallel\alpha}^2 = \mathbf{P}_{\parallel}^{\alpha} e^2 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 0 \\ -1-\alpha\tau \\ \tau-\alpha \end{bmatrix}$$

$$e_{\parallel\alpha}^3 = \mathbf{P}_{\parallel}^{\alpha} e^3 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} \tau-\alpha \\ 0 \\ 1+\alpha\tau \end{bmatrix} \qquad e_{\parallel\alpha}^4 = \mathbf{P}_{\parallel}^{\alpha} e^4 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 1+\alpha\tau \\ \tau-\alpha \\ 0 \end{bmatrix}$$

$$e_{\parallel\alpha}^5 = \mathbf{P}_{\parallel}^{\alpha} e^5 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} -1-\alpha\tau \\ \tau-\alpha \\ 0 \end{bmatrix} \qquad e_{\parallel\alpha}^6 = \mathbf{P}_{\parallel}^{\alpha} e^6 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} -\tau+\alpha \\ 0 \\ 1+\alpha\tau \end{bmatrix}.$$

3. Results

From the expressions above, the following results can be obtained.

(i) When $\alpha = 0$, the six vectors $e_{\parallel\alpha}^i$ are the six linear independent basis vectors of a perfect icosahedron:

$$e_{\parallel}^1 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 0 \\ 1 \\ \tau \end{bmatrix} \qquad e_{\parallel}^2 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 0 \\ -1 \\ \tau \end{bmatrix} \qquad e_{\parallel}^3 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} \tau \\ 0 \\ 1 \end{bmatrix}$$

$$e_{\parallel}^4 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} 1 \\ \tau \\ 0 \end{bmatrix} \qquad e_{\parallel}^5 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} -1 \\ \tau \\ 0 \end{bmatrix} \qquad e_{\parallel}^6 = \frac{1}{\sqrt{1+\tau^2}} \begin{bmatrix} -\tau \\ 0 \\ 1 \end{bmatrix}.$$

(ii) When $\alpha = (\tau - 1)/(\tau + 1) = 0.236$,

$$e_{\parallel\alpha}^1 = A \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \qquad e_{\parallel\alpha}^2 = A \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \qquad e_{\parallel\alpha}^3 = A \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

$$e_{\parallel\alpha}^4 = A \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \qquad e_{\parallel\alpha}^5 = A \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \qquad e_{\parallel\alpha}^6 = A \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

where

$$A = \frac{1}{\sqrt{1+\tau^2}} \frac{\tau+2}{\tau+1}.$$

It is clear that the six basis vectors $e_{\parallel\alpha}^i$ $(i = 1, \ldots, 6)$ are linearly dependent. There are only three linearly independent vectors $e_{\parallel\alpha}^1$, $e_{\parallel\alpha}^3$ and $e_{\parallel\alpha}^4$. There are the basis vectors of the FCC lattice. Then the reciprocal lattice of an icosahedron is transformed into one possessing m3m point group symmetry under the action of the soft-phason field.

(iii) When $\alpha = (K\tau - 1)/(\tau + K)$,

$$e_{\parallel\alpha}^1 = B \begin{bmatrix} 0 \\ K \\ 1 \end{bmatrix} \qquad e_{\parallel\alpha}^2 = B \begin{bmatrix} 0 \\ -K \\ 1 \end{bmatrix} \qquad e_{\parallel\alpha}^3 = B \begin{bmatrix} 1 \\ 0 \\ K \end{bmatrix}$$

$$e^4_{\|\alpha} = B\begin{bmatrix} K \\ 1 \\ 0 \end{bmatrix} \qquad e^5_{\|\alpha} = B\begin{bmatrix} -K \\ 1 \\ 0 \end{bmatrix} \qquad e^6_{\|\alpha} = B\begin{bmatrix} -1 \\ 0 \\ K \end{bmatrix}$$

where $K \neq 1$, and

$$B = \frac{1}{\sqrt{1+\tau^2}}\frac{\tau+2}{\tau+K}.$$

Then, the reciprocal lattice possesses m3 point group symmetry. Obviously, when K is a rational number, the $e^i_{\|\alpha}$ define the reciprocal lattice of a crystal. When K is an irrational number the $e^i_{\|\alpha}$ define a 3D incommensurate phase.

(iv) When $\alpha = \tau$,

$$e^1_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad e^2_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix} \qquad e^3_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$e^4_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad e^5_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix} \qquad e^6_{\|\alpha} = \sqrt{1+\tau^2}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

In this case, only three of the $e^i_{\|\alpha}$ are linearly independent: $e^1_{\|\alpha}$, $e^3_{\|\alpha}$ and $e^4_{\|\alpha}$. Obviously they are the basis vectors of the simple cubic lattice possessing m3m point group symmetry.

From the discussion above, one could come to some conclusions. Firstly, the phason strain W connects the reciprocal-lattice symmetries of the icosahedral quasi-crystal and crystal. The transformation of a recprocal lattice from an icosahedral quasi-crystal into a crystal can be obtained by projecting the 6D hyper-cubic lattice into the 3D hyperplane $Z^{\|}_3$ under the action of phason strain. Secondly, the effect of soft-phason strain on the hyperplane $Z^{\|}_3$ is to change its position (transformed into the hyperplane $Z^{\|\alpha}_3$) in 6D space, besides the origin of 6D space. Each value of α corresponds to one hyperplane, so that it can be used to describe phase transformations. In fact, all the theoretical results are in accordance with the studies of Al–Li–Cu quasi-crystals by the x-ray diffraction technique [10] and by the electron diffraction method [11]. These results confirm that there are several intermediate states between icosahedral quasi-crystals and cubic crystals. Further work is in progress.

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