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COMMENT

About hyperplane single rotation and phason strain equivalence in icosahedral and octagonal phases

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Abstract. We state here that the projection hyperplane change which is equivalent to the Al–Cu–Li icosahedral quasicrystal phason strain is, in fact, a single rotation in the 6D hyperspace. This approach is also valid for the octagonal phase and it generates, in a direct way, in both icosahedral and octagonal cases the quasicrystal–crystal intermediate phase density ratio. In the light of our picture of the unit cell it is clear which crystalline phases are realistically connected with the undistorted quasicrystalline phase.

In a recent paper, Zhenhong Mai and co-workers [1] show that the effect of the Al–Cu–Li icosahedral quasicrystal phason strain, which fits the symmetry distortions in their diffraction experiments [2], is equivalent to a hyperplane change in the projection-method approach. This hyperplane change can connect the undistorted quasicrystalline phase with crystalline ones through a continuous range of intermediate phases. On the other hand, we have essentially and independently reached the same last conclusion by means of a single rotation of the projection hyperplane in the hyperspace E^6 and directly working in the picture of the unit-cell [3].

In our above-mentioned work [3], undistorted icosahedral phase orthogonal projection matrices $\mathbf{P}^{\mathrm{I}}_{\parallel}$ and $\mathbf{P}^{\mathrm{I}}_{\perp}$ are given by

$$\begin{aligned}
\mathbf{P}^{\mathrm{I}}_{\parallel} &= \begin{bmatrix} c_{\mathrm{I}} & c_{\mathrm{I}} & 0 & 0 & -s_{\mathrm{I}} & s_{\mathrm{I}} \\ -s_{\mathrm{I}} & s_{\mathrm{I}} & c_{\mathrm{I}} & c_{\mathrm{I}} & 0 & 0 \\ 0 & 0 & -s_{\mathrm{I}} & s_{\mathrm{I}} & c_{\mathrm{I}} & c_{\mathrm{I}} \end{bmatrix} \\
\mathbf{P}^{\mathrm{I}}_{\perp} &= \begin{bmatrix} -s_{\mathrm{I}} & -s_{\mathrm{I}} & 0 & 0 & -c_{\mathrm{I}} & c_{\mathrm{I}} \\ -c_{\mathrm{I}} & c_{\mathrm{I}} & -s_{\mathrm{I}} & -s_{\mathrm{I}} & 0 & 0 \\ 0 & 0 & -c_{\mathrm{I}} & c_{\mathrm{I}} & -s_{\mathrm{I}} & -s_{\mathrm{I}} \end{bmatrix}
\end{aligned} \tag{1}$$

where $c_{\mathrm{I}} = \cos\theta_{\mathrm{I}}$, $s_{\mathrm{I}} = \sin\theta_{\mathrm{I}}$, $\theta_{\mathrm{I}} = \tan^{-1}(\tau - 1) = 31.7174°$ and $\tau = (1 + \sqrt{5})/2$. The general Bragg wavevector $G^{\mathrm{I}}_{\parallel}$ and its partner $G^{\mathrm{I}}_{\perp}$, which play a key role in the density-wave picture [1, 4–6], would be given by

$$
\begin{aligned}
G^{\mathrm{I}}_{\parallel} &= \pi \sum_{i=1}^{6} n_i u^{\mathrm{I}}_{\parallel i} = \pi \mathbf{P}^{\mathrm{I}}_{\parallel} L \\
G^{\mathrm{I}}_{\perp} &= \pi \sum_{i=1}^{6} n_i u^{\mathrm{I}}_{\perp i} = \pi \mathbf{P}^{\mathrm{I}}_{\perp} L
\end{aligned}
\tag{2}
$$

where

$$L = \sum_{i=1}^{6} n_i e_i \tag{3}$$

n_i are integers, $u^{\mathrm{I}}_{\parallel i} = \mathbf{P}^{\mathrm{I}}_{\parallel i} e_i$, $u^{\mathrm{I}}_{\perp i} = \mathbf{P}^{\mathrm{I}}_{\perp} e_i$, $\{e_i\}_{i=1,\ldots,6}$ is the canonical base of the hyperspace E^6 and the quasilattice parameter is taken as $a = 1$.

In order to describe the above-mentioned single rotation of the projection hyperplane in the 6D hyperspace [3], we change c_{I} by

$$c = \cos\theta = (1 + \alpha^2)^{-1/2}(c_{\mathrm{I}} - \alpha s_{\mathrm{I}}) \tag{4}$$

and s_{I} by

$$s = \sin\theta = (1 + \alpha^2)^{-1/2}(s_{\mathrm{I}} + \alpha c_{\mathrm{I}}) \tag{5}$$

where $\theta_{\mathrm{I}} - 90° < \theta < \theta_{\mathrm{I}} + 90°$, $-\infty < \alpha < \infty$, $\alpha = \tan(\theta - \theta_{\mathrm{I}})$ and $(\theta)_{\alpha=0} = \theta_{\mathrm{I}}$. By using this linear transformation, the static projection matrix $\mathbf{P}^{\mathrm{I}}_{\parallel}$ changes into the projection matrix $\mathbf{P}^{\theta}_{\parallel}$ on a rotatory hyperplane, given by

$$\mathbf{P}^{\theta}_{\parallel} = \begin{bmatrix} c & c & 0 & 0 & -s & s \\ -s & s & c & c & 0 & 0 \\ 0 & 0 & -s & s & c & c \end{bmatrix} = (1 + \alpha^2)^{-1/2}(\mathbf{P}^{\mathrm{I}}_{\parallel} + \alpha \mathbb{1} \mathbf{P}^{\mathrm{I}}_{\perp}) \tag{6}$$

where $\mathbb{1}$ is the identity matrix. $\alpha\mathbb{1}$ exactly corresponds with the second-rank tensor $\mathbf{M}$ of Zhenhong Mai and co-workers [1, 2] (taking into account our choice of vectors $u^{\mathrm{I}}_{\parallel i}, u^{\mathrm{I}}_{\perp i}, i = 1, \ldots, 6$).

According to (2) and (6), the wavevector $G^{\mathrm{I}}_{\parallel}$ changes into

$$G^{\theta}_{\parallel} = (1 + \alpha^2)^{-1/2}(G^{\mathrm{I}}_{\parallel} + \alpha G^{\mathrm{I}}_{\perp}) \tag{7}$$

when the projection hyperplane rotates. Thus, our single rotation performs an action equivalent to that of a phason linear field with strength α.

The descriptions of Zhenhong Mai and co-workers [1] and ours [3] coincide. In both of them, the perfect icosahedral symmetry is broken by three orthogonal planes defined by three twofold axes and the point subgroup $m\bar{3}$ is preserved. This symmetry rupture corresponds to the prolate and oblate rhombohedra splits, the first ones into 'green' (G) or 'red' (R) rhombohedra and the second ones into 'blue' (B) or 'yellow' (Y) rhombohedra [3]. In our description, vectors $u^{\theta}_{\parallel i} = \mathbf{P}^{\theta}_{\parallel} e_i$, $i = 1, \ldots, 6$, are normalised, which is necessary in order to avoid a variable scaling of the 6D hypercubic lattice [3, 7]. Zhenhong Mai and co-workers work in the density-wave picture and we work in the unit-cell picture. The above-mentioned coincidence is based on two facts: (i) the reciprocal lattice of a simple hypercubic lattice in direct space is also a simple hypercubic lattice in reciprocal space, and (ii) 'a star is eutactic if its symmetry group is irreducible' (p 261 of reference [7]), which permits us to connect our eutactic stars $\{u^{\mathrm{I}}_{\parallel i}\}_{i=1,\ldots,6}$ and $\{u^{\mathrm{I}}_{\perp i}\}_{i=1,\ldots,6}$ to the irreducible representations Γ_3 and $\Gamma_{3'}$ of the icosahedral group I [1].

The equivalence of the prior-projection hyperplane single rotation and linear phason strain can be translated in a straightforward manner for the octagonal phase. In this last case we project from hyperspace E^4 into the ordinary space E^2 [3]. The undistorted octagonal phase orthogonal projection matrices $\mathbf{P}^{\mathrm{O}}_{\parallel}$ and $\mathbf{P}^{\mathrm{O}}_{\perp}$ are given by

$$\begin{aligned} \mathbf{P}^{\mathrm{O}}_{\parallel} &= \begin{bmatrix} c_{\mathrm{O}} & c_{\mathrm{O}} & -s_{\mathrm{O}} & s_{\mathrm{O}} \\ -s_{\mathrm{O}} & s_{\mathrm{O}} & c_{\mathrm{O}} & c_{\mathrm{O}} \end{bmatrix} \\ \mathbf{P}^{\mathrm{O}}_{\perp} &= \begin{bmatrix} -s_{\mathrm{O}} & -s_{\mathrm{O}} & -c_{\mathrm{O}} & c_{\mathrm{O}} \\ -c_{\mathrm{O}} & c_{\mathrm{O}} & -s_{\mathrm{O}} & -s_{\mathrm{O}} \end{bmatrix} \end{aligned} \tag{8}$$

where $c_{\mathrm{O}} = \cos\theta_{\mathrm{O}}$, $s_{\mathrm{O}} = \sin\theta_{\mathrm{O}}$ and $\theta_{\mathrm{O}} = (\frac{1}{2})\tan^{-1}1 = 22.5°$. And, by the action of a phason linear field with strength α, the static projection matrix $\mathbf{P}^{\mathrm{O}}_{\parallel}$ changes into the projection matrix $\mathbf{P}^{\theta}_{\parallel}$ on a rotatory hyperplane (ordinary plane here), given by

$$\mathbf{P}^{\theta}_{\parallel} = \begin{bmatrix} c & c & -s & s \\ -s & s & c & c \end{bmatrix} = (1+\alpha^2)^{-1/2}(\mathbf{P}^{\mathrm{O}}_{\parallel} + \alpha\mathbb{1}\mathbf{P}^{\mathrm{O}}_{\perp}) \tag{9}$$

where $c = \cos\theta, s = \sin\theta, \alpha = \tan(\theta - \theta_{\mathrm{O}}), \theta_{\mathrm{O}} - 90° < \theta < \theta_{\mathrm{O}} + 90°, -\infty < \alpha < \infty$ and $(\theta)_{\alpha=0} = \theta_{\mathrm{O}}$.

Here, the linear phason strain splits the 45° rhombi into rhombi A or B [3].

The normalisation factor $(1+\alpha^2)^{-1/2}$ plays a central role in the calculation of the quasicrystal–crystal intermediate phase density ratio. In the case of the icosahedral phase, we obtain

$$\rho/\rho_{\mathrm{I}} = (1+\alpha^2)^{3/2} = 1/\cos^3(\theta - \theta_{\mathrm{I}}) \tag{10}$$

where ρ_{I} is the undistorted icosahedral phase density and ρ is that for the distorted icosahedral phase. In the case of the octagonal phase, we obtain

$$\rho/\rho_{\mathrm{O}} = 1 + \alpha^2 = 1/\cos^2(\theta - \theta_{\mathrm{O}}) \tag{11}$$

where ρ_{O} is the undistorted octagonal phase density and ρ is that for the distorted octagonal phase. From equations (10) and (11) the relative frequencies of occurrence of the different generalised types of tile can be calculated in the two above-mentioned cases [3].

In the light of our unit-cell picture [3], it is clear that the phason strain and hyperplane rotation models are restricted to the tilings range where the tiles do not overlap. In other words, the range of quasilattice with tiles overlapping is physically forbidden. That is, only the range $0° \leqslant \theta \leqslant 45°$ (or, equivalently, $-\tau^{-1} \leqslant \alpha \leqslant \tau^{-3}$) for the icosahedral case, and the range $0° \leqslant \theta \leqslant 45°$ (or, equivalently, $1 - \sqrt{2} \leqslant \alpha \leqslant \sqrt{2} - 1$) for the octagonal case are permitted. So, the simple cubic phase proposed by Zhenhong Mai and co-workers for $\alpha = \tau$ ($\theta = 90°$) [1] is not realistic because there is a gap of quasilattices with tiles overlapping which separates the above-mentioned potential simple cubic phase from the undistorted icosahedral one ($\alpha = 0$, $\theta = 31.7174°$). However, there is other simple cubic phase for $\alpha = -\tau^{-1}$ ($\theta = 0°$) which is connected in a continuous way (without tiles overlapping) with the perfect icosahedral one [3]. In any case, the FCC phase for $\alpha = \tau^{-3} = 0.236$ ($\theta = 45°$) [1, 3] is the one that is physically closest to the undistorted icosahedral phase. In fact, Zhenhong Mai and co-workers have obtained experimentally an intermediate phase with $\alpha = 0.22$ ($\theta = 44.1248°$) that almost coincides with the FCC phase [2].

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