Diffuse scattering from octagonal quasicrystals

1999 J. Phys.: Condens. Matter 11 1211

(http://iopscience.iop.org/0953-8984/11/5/009)

J. Phys.: Condens. Matter **11** (1999) 1211–1223. Printed in the UK PII: S0953-8984(99)94479-X

Diffuse scattering from octagonal quasicrystals

Jianlin Lei, Chengzheng Hu, Renhui Wang† and Di-hua Ding
Department of Physics, Wuhan University, Wuhan 430072, People's Republic of China

Received 22 May 1998, in final form 27 October 1998

Abstract. Explicit formulae for thermal diffuse scattering from octagonal quasicrystals have been derived in terms of elastic constants. Contours of constant diffuse scattering intensity are calculated. The anisotropic peak shapes vary greatly even for Bragg spots aligned with a given direction in reciprocal space. Diffuse scattering patterns in the plane perpendicular to a given zone axis are associated with corresponding specific elastic constants. Analysis of peak shapes can be used to acquire numerical values of elastic constants if diffuse scattering patterns can be measured precisely.

1. Introduction

The discovery of Al–Mn alloy with icosahedral symmetry (Shechtman *et al* 1984), followed promptly by other forbidden symmetries, opened rapidly a new field in condensed matter physics and crystallography. The striking characteristic of quasicrystals is the existence of sharp Bragg peaks. However, distortion and peak broadening observed in diffraction patterns revealed some systematic deviations from the ideal quasicrystal model (Bancel *et al* 1985, Bancel and Heiney 1986). How strains in phonon and phason variables or quenched dislocations can lead to these experimental observations has been discussed (Lubensky *et al* 1986, Horn *et al* 1986). Socolar and Wright (1987) have examined the shapes of Bragg spots observed in icosahedral phases and reproduced the peak shapes by the superposition of uniform phason strains. Jaric and Nelson (1988) have developed an alternative theory of diffuse scattering from incommensurate crystals and quasicrystals due to spatially fluctuating thermal and quenched strains and applied their derived general formulae to a specific case of icosahedral quasicrystals according to elastic properties of icosahedral quasicrystals which have been the focus of many theoretical works (Levine *et al* 1985, Lubensky *et al* 1985, Bak 1985a, b). With the help of this theory, the onset of hydrodynamic instability of icosahedral phases has been discussed (Widom 1991, Ishii 1992); the diffuse scattering located close to Bragg reflections has been studied as a function of the temperature on a single grain of the Al–Pd–Mn icosahedral phase using elastic neutron scattering and the ratio of two phason elastic constants was obtained (de Boisseau *et al* 1995, Boudard *et al* 1996).

Kuo and his colleagues observed experimentally octagonal quasicrystals in $Ni_{10}SiV_{15}$ and $Cr_5Ni_3Si_2$ (Wang *et al* 1987), in Mn_4Si (Cao *et al* 1988), in $Al_3Mn_{82}Si_{15}$ (Wang *et al* 1988) and in Fe–Mn–Si (Wang and Kuo 1988) which are all metastable. Elastic properties of planar quasicrystals with eightfold symmetry have been discussed in the literature (Socolar 1989, Ding *et al* 1993, Hu *et al* 1993). Recently, some investigators have restricted attention to two-dimensional (2D) quasicrystals including octagonal quasicrystals (Yang *et al* 1995,

† Corresponding author.

Hu *et al* 1996, 1997). Based on the 5D crystallographic symmetry operations listed by Janssen (1992), they have derived all possible point groups of 2D quasicrystals of rank 5 and calculated the numbers of independent fourth-rank elastic constants of 2D quasicrystals with group representation theory. Here and hereafter, a 2D quasicrystal refers not to a real plane but to a 3D solid with 2D quasiperiodic and 1D periodic structure.

The purpose of this paper was to investigate diffuse scattering from octagonal quasicrystals theoretically. Point groups, Laue classes and elastic properties of octagonal quasicrystals are summarized in section 2. Diffuse scattering from octagonal quasicrystals is formulated in section 3. Contours of constant diffuse scattering intensity are illustrated and discussion of the results are given in section 4. The coordinate systems which we use for octagonal quasicrystals are given in the appendix.

2. Point groups, Laue classes and elastic properties of octagonal quasicrystals

In this section we will illustrate the determination of explicit forms of invariant terms in the elastic energy and elastic constant tensor for the octagonal system. We would like to limit the brief description of this method to a minimum necessary for the calculation. A more detailed discussion can be found in the literature (Hu *et al* 1993, 1996, 1997, Yang *et al* 1995).

If an analytic expression of the elastic free energy is possible, it will be quadratic in the special gradients of phonon displacements $\boldsymbol{u}^{\parallel}$ and phason displacements $\boldsymbol{u}^{\perp}$ at long wavelength when it is expanded in terms of the Taylor series to the second order. Since the elastic energy is a scalar quantity, each individual term in it mush be invariant under all of the point group operations of the structure. In order to construct these quadratic invariants, we can invoke the group representation theory. As an example, we consider the point group $8mm(\mathrm{D}_8)$ generated by a eightfold rotation α and a mirror β, which can be represented by

$$\Gamma(\alpha)\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \qquad \Gamma(\beta)=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{2.1}$$

Repeated application of these two matrices generates a representation of the point group $8mm$, which we denote Γ. This representation is reducible. The reduction is

$$\Gamma = \Gamma_5 + \Gamma_1 + \Gamma_7. \tag{2.2}$$

It follows that $\boldsymbol{u}^{\parallel}$ transforms under $\Gamma_5 + \Gamma_1$ and $\boldsymbol{u}^{\perp}$ transforms under Γ_7. Therefore, the displacement gradients $\partial_j \boldsymbol{u}_i^{\parallel}$ $(i, j = 1, 2, 3)$ and $\partial_j u_i^{\perp}$ $(i = 1, 2, j = 1, 2, 3)$ transform according to their respective direct product representation. It should be noted that $\boldsymbol{u}^{\parallel}$ is a three-component vector while $\boldsymbol{u}^{\perp}$ a two-component vector, and both of them are the functions of the position vector in the physical space only. For the phonon field, the nine components of $\partial_j \boldsymbol{u}_i^{\parallel}$ transform under

$$(\Gamma_5 + \Gamma_1) \times (\Gamma_5 + \Gamma_1) = 2\Gamma_1 + 2\Gamma_5 + \Gamma_2 + \Gamma_6. \tag{2.3}$$

Among them the antisymmetric components $\partial_1 u_2^{\parallel} - \partial_2 u_1^{\parallel}$, $\partial_2 u_3^{\parallel} - \partial_3 u_2^{\parallel}$, $\partial_3 u_1^{\parallel} - \partial_1 u_3^{\parallel}$ transform under $\Gamma_5 + \Gamma_2$ corresponding to rigid rotations, which do not change the elastic energy. The symmetric components $\partial_1 u_1^{\parallel} + \partial_2 u_2^{\parallel}$ and $\partial_3 u_3^{\parallel}$ transform under Γ_1 (the identity representation), from which it follows that there are three quadratic invariants:

$$(E_{11} + E_{22})^2,\ E_{33}^2,\ (E_{11} + E_{22})E_{33} \tag{2.4}$$

where $E_{ij} = \frac{1}{2}(\partial_j u_1^\parallel + \partial_i u_j^\parallel)$ is used. The pairs $(\partial_1 u_1^\parallel - \partial_2 u_2^\parallel, \partial_1 u_2^\parallel + \partial_2 u_1^\parallel)$ and $(\partial_3 u_1^\parallel + \partial_1 u_3^\parallel, \partial_3 u_2^\parallel + \partial_2 u_3^\parallel)$ span the 2D irreducible representations Γ_6 and Γ_5 respectively. Since Γ_1 occurs once and only once in the products $\Gamma_6 \times \Gamma_6$ and $\Gamma_5 \times \Gamma_5$, it is obvious that

$$(E_{11} - E_{22})^2 + (2E_{12})^2, E_{13}^2 + E_{23}^2 \tag{2.5}$$

are two invariants. From equations (2.4) and (2.5), it follows that associated with the phonon field there are five quadratic invariants and five independent elastic constants

$$C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66} = \tfrac{1}{2}(C_{11} - C_{12}). \tag{2.6}$$

For the phason field six components of $\partial_j u_i^\perp$ transform under

$$(\Gamma_5 + \Gamma_1) \times \Gamma_7 = \Gamma_3 + \Gamma_4 + \Gamma_6 + \Gamma_7. \tag{2.7}$$

The components $\partial_1 u_1^\perp - \partial_2 u_2^\perp$ and $\partial_1 u_2^\perp + \partial_2 u_1^\perp$ transform under Γ_3 and Γ_4 respectively, from which it follows that there are two quadratic invariants:

$$(\partial_1 u_1^\perp - \partial_2 u_2^\perp)^2, (\partial_1 u_2^\perp + \partial_2 u_1^\perp)^2. \tag{2.8}$$

The pairs $(\partial_1 u_1^\perp + \partial_2 u_2^\perp, \partial_1 u_2^\perp - \partial_2 u_1^\perp)$ and $(\partial_3 u_1^\perp, \partial_3 u_2^\perp)$ span the 2D irreducible representations Γ_6 and Γ_7 respectively. Thus, we can obtain two quadratic invariants:

$$(\partial_1 u_1^\perp + \partial_2 u_2^\perp)^2 + (\partial_1 u_2^\perp - \partial_2 u_1^\perp)^2, (\partial_3 u_1^\perp)^2 + (\partial_3 u_2^\perp)^2. \tag{2.9}$$

From equations (2.8) and (2.9), it follows that associated with the phason field there are four quadratic invariants and four independent elastic constants. Nonvanishing elastic constants are

$$\begin{aligned} &K_{1111} = K_{2222} = K_1, K_{1122} = K_{2211} = K_2, K_{1221} = K_{2112} = K_3, \\ &\qquad K_{1313} = K_{2323} = K_4, K_{1212} = K_{2121} = K_1 + K_2 + K_3. \end{aligned} \tag{2.10}$$

Moreover, notice that the irreducible representation Γ_6 occurs in both of the reduction equations (2.3) and (2.7). This means that there exists an invariant

$$(E_{11} - E_{22})(\partial^\perp u_1^\perp + \partial_2 u_2^\perp) + 2E_{12}(\partial_1 u_2^\perp - \partial_2 u_1^\perp) \tag{2.11}$$

coupling $\boldsymbol{u}^\parallel$ and $\boldsymbol{u}^\perp$. The nonvanishing elastic constant is

$$R_{1111} = R_{1122} = -R_{2211} = -R_{2222} = R_{1221} = R_{2121} = -R_{1212} = -R_{2112} = R_1. \tag{2.12}$$

Therefore, it can be seen that there are ten quadratic invariants and hence ten independent elastic constants for $8mm$. Among them five elastic constants are associated with the phonon field, four with the phason field and one with the phonon–phason coupling.

In the same way we can find all invariants and independent elastic constants for 8 (C_8) symmetry. There are twelve quadratic invariants and hence twelve independent elastic constants. Among them ten elastic constants are the same as those for $8mm$; the other two are the nonvanishing phason elastic constant

$$K_{1112} = K_{1211} = K_{1121} = K_{2111} = -K_{2212} = -K_{1222} = -K_{2221} = -K_{2122} = K_5 \tag{2.13}$$

and the phonon–phason coupling elastic constant

$$R_{1112} = -R_{1121} = -R_{2212} = R_{2221} = R_{1211} = R_{2111} = R_{1222} = R_{2122} = R_2. \tag{2.14}$$

The octagonal system has seven point groups divided into two Laue classes which we term Laue classes 15 and 16 respectively. Laue class 15 includes 8, $\bar{8}$ and $8/m$ while Laue class 16 includes $8mm$, 822, $\bar{8}m2$ and $8/mmm$. Elastic properties possess an inherent centrosymmetry. Therefore, all point groups belonging to the same Laue class possess the same elastic properties.

3. Formulae for diffuse scattering from octagonal quasicrystals

3.1. General formulae for diffuse scattering from quasicrystals

Here we derive general formulae for diffuse scattering from quasicrystals by a method similar to that used for ordinary crystals (Wooster 1962). In higher-dimensional description of quasicrystals the density of a quasicrystal can be represented by

$$\rho^{\parallel}(\boldsymbol{x}^{\parallel}) = \rho(\boldsymbol{x}^{\parallel}, \boldsymbol{x}^{\perp} = \mathbf{0}) \tag{3.1}$$

where ρ is the corresponding density in d-dimensional embedding space. Furthermore,

$$\rho(\boldsymbol{x}) = \rho_0(\boldsymbol{x}) - \Delta\rho(\boldsymbol{x}) = \rho_0(\boldsymbol{x}) - \boldsymbol{\nabla}\cdot[\rho_0(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}^{\parallel})] \tag{3.2}$$

where $\rho(\boldsymbol{x})$ corresponds to the density in the hyperspace of a disordered quasicrystal and $\rho_0(\boldsymbol{x})$ that of a perfect quasicrystal, $\boldsymbol{u}(\boldsymbol{x}^{\parallel}) = \int \boldsymbol{u}(\boldsymbol{p}^{\parallel})\,\mathrm{e}^{\mathrm{i}(\boldsymbol{p}^{\parallel}\cdot\boldsymbol{x}^{\parallel}-\omega(\boldsymbol{p}^{\parallel})t)}\,\mathrm{d}^3p^{\parallel}$ is the d-dimensional displacement field mentioned in the preceding section and $\Delta\rho(\boldsymbol{x})$ is the density decrease at the position $\boldsymbol{x}$ caused by the displacement field $\boldsymbol{u}(\boldsymbol{x}^{\parallel})$. This equation can be regarded as an extension of the ordinary equation of continuity to the higher-dimensional case. Therefore, equation (3.1) can be replaced by

$$\rho^{\parallel}(\boldsymbol{x}^{\parallel}) = \rho_0^{\parallel}(\boldsymbol{x}^{\parallel}) - \Delta\rho^{\parallel}(\boldsymbol{x}^{\parallel}). \tag{3.3}$$

Furthermore, $\rho_0(\boldsymbol{x})$ can be written as

$$\rho_0(\boldsymbol{x}) = \sum_{\boldsymbol{R}} \delta(\boldsymbol{x}-\boldsymbol{R}) * \rho_c(\boldsymbol{x}) \tag{3.4}$$

where $\boldsymbol{R}$ is a hyperlattice point, $*$ means convolution and $\rho_c(\boldsymbol{x})$ denotes the density in a unit hypercell. The Fourier transform of $\rho_0(\boldsymbol{x})$ is

$$\Phi_0(\boldsymbol{q}) = \int \rho_0(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\,\mathrm{d}^dx = \sum_{\boldsymbol{R}} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}}F(\boldsymbol{q}) = \frac{(2\pi)^d}{v_c}\sum_{\boldsymbol{Q}}\delta(\boldsymbol{q}-\boldsymbol{Q})F(\boldsymbol{Q}) \tag{3.5}$$

where v_c is the volume of the unit hypercell, $\boldsymbol{Q}$ is the reciprocal hyperlattice vector and

$$F(\boldsymbol{q}) = \int \rho_c(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\,\mathrm{d}^dx \tag{3.6}$$

is the structure factor of the unit hypercell. From equation (3.5) $\rho_0(\boldsymbol{x})$ can also be written in the form of the inverse Fourier transform of $\Phi_0(\boldsymbol{q})$,

$$\rho_0(\boldsymbol{x}) = \frac{1}{(2\pi)^d}\int \Phi_0(\boldsymbol{q})\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\,\mathrm{d}^dq = \frac{1}{v_c}\sum_{\boldsymbol{Q}} F(\boldsymbol{Q})\,\mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{x}}. \tag{3.7}$$

Substituting this expression into equation (3.2), and after writing $\Delta\rho(\boldsymbol{x})$ in terms of the Fourier transform $\boldsymbol{u}(\boldsymbol{p}^{\parallel})$, we have

$$\Delta\rho(\boldsymbol{x}) = \frac{\mathrm{i}}{v_c}\sum_{\boldsymbol{Q}} F(\boldsymbol{Q})\int(\boldsymbol{Q}+\boldsymbol{p}^{\parallel})\cdot\boldsymbol{u}(\boldsymbol{p}^{\parallel})\,\mathrm{e}^{\mathrm{i}(\boldsymbol{Q}+\boldsymbol{p}^{\parallel})\cdot\boldsymbol{x}}\,\mathrm{d}^3p^{\parallel}. \tag{3.8}$$

The Fourier transform of $\Delta\rho(\boldsymbol{x})$ is

$$\Delta\Phi(\boldsymbol{q}) = \int \Delta\rho(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\,\mathrm{d}^dx = \mathrm{i}\frac{(2\pi)^d}{v_c}\sum_{\boldsymbol{Q}} F(\boldsymbol{Q})\int(\boldsymbol{Q}+\boldsymbol{p}^{\parallel})\cdot\boldsymbol{u}(\boldsymbol{p}^{\parallel})\delta(\boldsymbol{q}-\boldsymbol{Q}-\boldsymbol{p}^{\parallel})\,\mathrm{d}^3p^{\parallel}. \tag{3.9}$$

Since the Fourier transform of a cut is equal to a projection of a Fourier transform, the Fourier transform of $\rho_0^{\parallel}(\boldsymbol{x}^{\parallel})$ is

$$\Phi_0^{\parallel}(\boldsymbol{q}^{\parallel}) = \int \Phi_0(\boldsymbol{q})\,\mathrm{d}^{d-3}q^{\perp} = \frac{(2\pi)^d}{v_c}\sum_{\boldsymbol{Q}}\delta^{\parallel}(\boldsymbol{q}^{\parallel}-\boldsymbol{Q}^{\parallel})F(\boldsymbol{Q}). \tag{3.10}$$

Similarly, the Fourier transform of $\Delta\rho^{\parallel}(\boldsymbol{x}^{\parallel})$ is

$$\Delta\Phi^{\parallel}(\boldsymbol{q}^{\parallel}) = \int \Delta\Phi(\boldsymbol{q})\,\mathrm{d}^{d-3}q^{\perp} = \mathrm{i}\frac{(2\pi)^d}{v_c}\sum_{\boldsymbol{Q}} F(\boldsymbol{Q})(\boldsymbol{q}^{\parallel} + \boldsymbol{Q}^{\perp})\cdot\boldsymbol{u}(\boldsymbol{q}^{\parallel} - \boldsymbol{Q}^{\parallel}). \tag{3.11}$$

Therefore, the observed intensity is

$$\begin{aligned} I(q^{\parallel}) &= |\Phi^{\parallel}(q^{\parallel})|^2 = |\Phi_0^{\parallel}(q_0^{\parallel}) + \Delta\Phi^{\parallel}(q^{\parallel})|^2 \\ &= |\Phi_0^{\parallel}(q_0^{\parallel})|^2 + 2\,\mathrm{Re}(\Phi_0^{\parallel}(q_0^{\parallel})\Delta\Phi^{\parallel}(q^{\parallel})) + |\Delta\Phi^{\parallel}(q^{\parallel})|^2 \end{aligned} \tag{3.12}$$

where the first term is independent of $\boldsymbol{u}$, the second term is linear in $\boldsymbol{u}$ and the third term quadratic in $\boldsymbol{u}$. Since $\boldsymbol{u}$ is a thermodynamic quantity, we must carry out the statistical average. After the average over the probability distribution of $\boldsymbol{u}$ the surviving terms are

$$I_{\mathrm{Bragg}}(\boldsymbol{q}^{\parallel}) = |\Phi_0^{\parallel}(\boldsymbol{q}^{\parallel})|^2 = \frac{V}{(2\pi)^3}\frac{(2\pi)^{2d}}{v_c^2}\sum_{\boldsymbol{Q}} \delta^{\parallel}(\boldsymbol{q}^{\parallel} - \boldsymbol{Q}^{\parallel})|F(\boldsymbol{Q})|^2 \tag{3.13}$$

and

$$I_{\mathrm{ds}}(\boldsymbol{q}^{\parallel}) = |\Delta\Phi^{\parallel}(\boldsymbol{q}^{\parallel})|^2 = \frac{(2\pi)^{2d}}{v_c^2}\sum_{\boldsymbol{Q}} |F(\boldsymbol{Q})|^2|(\boldsymbol{q}^{\parallel} + \boldsymbol{Q}^{\perp})\cdot\boldsymbol{u}(\boldsymbol{q}^{\parallel} - \boldsymbol{Q}^{\parallel})|^2 \tag{3.14}$$

where V is the volume of the studied quasicrystal and the Debye–Waller factor is contained in $|F(\boldsymbol{Q})|^2$. The former gives the Bragg scattering intensity and the latter the diffuse scattering intensity. It follows from equations (3.13) and (3.14) that the integrated intensity of Bragg scattering around a particular Bragg spot $\boldsymbol{Q}^{\parallel}$ is

$$I_{\mathrm{Bragg}}(\boldsymbol{Q}^{\parallel}) = \frac{V}{(2\pi)^3}\frac{(2\pi)^{2d}}{v_c^2}|F(\boldsymbol{Q})|^2 \tag{3.15}$$

and sufficiently near a particular Bragg spot $\boldsymbol{Q}^{\parallel}$, the diffuse scattering intensity is

$$I_{\mathrm{ds}}(\boldsymbol{Q}^{\parallel} + \boldsymbol{p}^{\parallel}) \approx \frac{(2\pi)^{2d}}{v_c^2}|F(\boldsymbol{Q})|^2|\boldsymbol{Q}\cdot\boldsymbol{u}(\boldsymbol{p}^{\parallel})|^2 \tag{3.16}$$

since the contributions from other Bragg spots may be neglected. In order to find the explicit expression for $\boldsymbol{u}(\boldsymbol{p}^{\parallel})$, we can employ the generalized elasticity theory of quasicrystals (Ding *et al* 1993) according to which the equations of motion are

$$\begin{aligned} C_{ijkl}\frac{\partial^2 u_k^{\parallel}(\boldsymbol{x}^{\parallel})}{\partial x_j\partial x_l} + R_{ijkl}\frac{\partial^2 u_k^{\perp}(\boldsymbol{x}^{\parallel})}{\partial x_j\partial x_l} &= \mu\frac{\partial^2 u_i^{\parallel}(\boldsymbol{x}^{\parallel})}{\partial^2 t} \\ R_{klij}\frac{\partial^2 u_k^{\parallel}(\boldsymbol{x}^{\parallel})}{\partial x_j\partial x_l} + K_{ijkl}\frac{\partial^2 u_k^{\perp}(\boldsymbol{x}^{\parallel})}{\partial x_j\partial x_l} &= \mu\frac{\partial^2 u_i^{\perp}(\boldsymbol{x}^{\parallel})}{\partial^2 t} \end{aligned} \tag{3.17}$$

or, in terms of the Fourier transform $\boldsymbol{u}(\boldsymbol{p}^{\parallel})$,

$$\begin{aligned} C_{ijkl}p_j^{\parallel}p_l^{\parallel}u_k^{\parallel}(\boldsymbol{p}^{\parallel}) + R_{ijkl}p_j^{\parallel}p_l^{\parallel}u_k^{\perp}(\boldsymbol{p}^{\parallel}) &= \mu\omega^2(\boldsymbol{p}^{\parallel})u_i^{\parallel}(\boldsymbol{p}^{\parallel}) \\ R_{klij}p_j^{\parallel}p_l^{\parallel}u_k^{\parallel}(\boldsymbol{p}^{\parallel}) + K_{ijkl}p_j^{\parallel}p_l^{\parallel}u_k^{\perp}(\boldsymbol{p}^{\parallel}) &= \mu\omega^2(\boldsymbol{p}^{\parallel})u_i^{\perp}(\boldsymbol{p}^{\parallel}) \end{aligned} \tag{3.18}$$

which can be written in the matrix form

$$\begin{bmatrix} \mathsf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel}) & \mathsf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel}) \\ \mathsf{A}^{\perp,\parallel}(\boldsymbol{p}^{\parallel}) & \mathsf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel}) \end{bmatrix}\begin{bmatrix} \boldsymbol{u}^{\parallel}(\boldsymbol{p}^{\parallel}) \\ \boldsymbol{u}^{\perp}(\boldsymbol{p}^{\parallel}) \end{bmatrix} = \mu\omega^2(\boldsymbol{p}^{\parallel})\begin{bmatrix} \boldsymbol{u}^{\parallel}(\boldsymbol{p}^{\parallel}) \\ \boldsymbol{u}^{\perp}(\boldsymbol{p}^{\parallel}) \end{bmatrix}$$

with

$$[\mathsf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})]_{ik} = C_{ijkl}\,p_j^{\parallel}p_l^{\parallel}$$
$$[\mathsf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel})]_{ik} = K_{ijkl}\,p_j^{\parallel}p_l^{\parallel} \tag{3.19}$$
$$[\mathsf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel})]_{ik} = [\mathsf{A}^{\perp,\parallel}(\boldsymbol{p}^{\parallel})]_{ki} = R_{ijkl}\,p_j^{\parallel}p_l^{\parallel}.$$

Equation (3.19) can be regarded as an extension of Christoffel's equation from the case of ordinary crystals to that of quasicrystals.

Letting

$$\mathsf{A}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} \mathsf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel}) & \mathsf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel}) \\ \mathsf{A}^{\perp,\parallel}(\boldsymbol{p}^{\parallel}) & \mathsf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel}) \end{bmatrix} \qquad \lambda(\boldsymbol{p}^{\parallel}) = \mu\omega^2(\boldsymbol{p}^{\parallel}) \tag{3.20}$$

we have

$$\mathsf{A}(\boldsymbol{p}^{\parallel})\cdot\boldsymbol{u}(\boldsymbol{p}^{\parallel}) = \lambda(\boldsymbol{p}^{\parallel})\boldsymbol{u}(\boldsymbol{p}^{\parallel}). \tag{3.21}$$

This is a standard eigenvalue equation for the hydrodynamic matrix $\mathsf{A}(\boldsymbol{p}^{\parallel})$ (Jennings 1977). For a given wavevector, there are d eigenvalues $\lambda_{(\alpha)}(\boldsymbol{p}^{\parallel})$ and d unit eigenvectors $\boldsymbol{e}_{(\alpha)}(\boldsymbol{p}^{\parallel})$. Then

$$\lambda_{(\alpha)}(\boldsymbol{p}^{\parallel}) = \mu\omega^2_{(\alpha)}(\boldsymbol{p}^{\parallel}) \qquad \boldsymbol{u}_{(\alpha)}(\boldsymbol{p}^{\parallel}) = \xi_{(\alpha)}(\boldsymbol{p}^{\parallel})\boldsymbol{e}_{(\alpha)}(\boldsymbol{p}^{\parallel}) \qquad (\alpha = 1, 2, \ldots, d) \tag{3.22}$$

where $\xi_{(\alpha)}(\boldsymbol{p}^{\parallel})$ denotes the amplitude of $\boldsymbol{u}_{(\alpha)}(\boldsymbol{p}^{\parallel})$. The scattering intensities due to the d elastic waves simply add because the d scattered radiations are incoherent. Therefore, equation (3.16) should be replaced by

$$I_{\mathrm{ds}}(\boldsymbol{Q}^{\parallel}+\boldsymbol{p}^{\parallel}) = \frac{(2\pi)^{2d}}{v_c^2}|F(\boldsymbol{Q})|^2\sum_{\alpha}|\xi_{(\alpha)}(\boldsymbol{p}^{\parallel})|^2|\boldsymbol{Q}\cdot\boldsymbol{e}_{(\alpha)}(\boldsymbol{p}^{\parallel})|^2. \tag{3.23}$$

To calculate the thermodynamic average in equation (3.23), we can employ the energy equipartition theorem which leads to

$$\frac{1}{2}\mu V\left|\frac{(2\pi)^3}{V}\xi_{(\alpha)}(\boldsymbol{p}^{\parallel})\right|^2\omega^2_{(\alpha)}(\boldsymbol{p}^{\parallel}) = \frac{1}{2}k_BT \tag{3.24}$$

where T is temperature and k_B is the Boltzmann constant. Using the value of $|\xi_{(\alpha)}(\boldsymbol{p}^{\parallel})|^2$ calculated from equation (3.24), and using equations (3.15) and (3.23), we find that

$$I_{\mathrm{ds}}(\boldsymbol{Q}^{\parallel}+\boldsymbol{p}^{\parallel}) = \frac{k_BT}{(2\pi)^3}\sum_{\alpha}\frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_{(\alpha)}(\boldsymbol{p}^{\parallel}))(\boldsymbol{e}_{(\alpha)}(\boldsymbol{p}^{\parallel})\cdot\boldsymbol{Q})}{\lambda_{(\alpha)}(\boldsymbol{p}^{\parallel})}I_{\mathrm{Bragg}}(\boldsymbol{Q}^{\parallel}). \tag{3.25}$$

Notice that (Jennings 1977)

$$\frac{e_{(\alpha)p}(\boldsymbol{p}^{\parallel})e_{(\alpha)q}(\boldsymbol{p}^{\parallel})}{\lambda_{(\alpha)}(\boldsymbol{p}^{\parallel})} = [\mathsf{A}^{-1}(\boldsymbol{p}^{\parallel})]_{pq} \tag{3.26}$$

where subscripts p and q denote the components. We can immediately write out

$$I_{\mathrm{ds}}(\boldsymbol{Q}^{\parallel}+\boldsymbol{p}^{\parallel}) = \frac{k_BT}{(2\pi)^3}\boldsymbol{Q}\cdot\mathsf{A}^{-1}(\boldsymbol{p}^{\parallel})\cdot\boldsymbol{Q}\cdot I_{\mathrm{Bragg}}(\boldsymbol{Q}^{\parallel}). \tag{3.27}$$

The result coincides with that given by Jaric and Nelson (1988) except for a constant coefficient.

If the phasons drop out of thermal equilibrium at an elevated temperature T_q, then at a lower temperature T, phonons will equilibrate in the presence of a quenched phason displacement field. This situation has been examined by Jaric and Nelson (1988) and Lei *et al* (1999) and it has been concluded (Lei *et al* 1999) that $\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})$, $\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel})$ and $\mathbf{A}^{\perp,\parallel}(\boldsymbol{p}^{\parallel})$ blocks are still given by equation (3.19) but the $\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel})$ block should be modified by

$$\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel}) = \frac{T}{T_q}\{\mathbf{A}_q^{\perp,\perp}(\boldsymbol{p}^{\parallel}) - \mathbf{A}_q^{\perp,\parallel}(\boldsymbol{p}^{\parallel})\cdot[\mathbf{A}_q^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})]^{-1}\cdot\mathbf{A}_q^{\parallel,\perp}(\boldsymbol{p}^{\parallel})\} + \mathbf{A}^{\perp,\parallel}(\boldsymbol{p}^{\parallel})\cdot[\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})]^{-1}\cdot\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel}) \tag{3.28}$$

where the subscript q means that the values of the elastic constants at T_q should be used. It should be emphasized that matrix $\mathbf{A}(\boldsymbol{p}^{\parallel})$ is associated not only with phonon and phonon–phonon coupling elastic constants $C_{ijkl}(T)$, $R_{ijkl}(T)$ at T, but also with all of the elastic constants $C_{ijkl}(T_q)$, $K_{ijkl}(T_q)$ and $R_{ijkl}(T_q)$ at T_q. Obviously, equation (3.28) will be reduced to that defined in equation (3.19) if $T = T_q$, which is physically reasonable.

3.2. *Explicit expressions for a specific case of octagonal quasicrystals*

It has been pointed out in section 2 that all point groups belonging to the same Laue class possess the same elastic properties due to the inherent centrosymmetry of elastic properties. Therefore, matrix $\mathbf{A}(\boldsymbol{p}^{\parallel})$ is identical for all point groups belonging to the same Laue class. From elastic properties of octagonal quasicrystals, explicit expressions of $\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})$, $\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel})$ and $\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel})$ blocks for each Laue class of octagonal system can be easily obtained.

3.2.1. Laue class 15. In this case, $\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})$, $\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel})$ and $\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel})$ blocks are given by

$$\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} C_{11}p_1^{\parallel 2} + C_{66}p_2^{\parallel 2} + C_{44}p_3^{\parallel 2} & (C_{11} - C_{66})p_1^{\parallel}p_2^{\parallel} & (C_{44} + C_{13})p_1^{\parallel}p_3^{\parallel} \\ (C_{11} - C_{66})p_1^{\parallel}p_2^{\parallel} & C_{66}p_1^{\parallel 2} + C_{11}p_2^{\parallel 2} + C_{44}p_3^{\parallel 2} & (C_{44} + C_{13})p_2^{\parallel}p_3^{\parallel} \\ (C_{44} + C_{13})p_1^{\parallel}p_3^{\parallel} & (C_{44} + C_{13})p_2^{\parallel}p_3^{\parallel} & C_{44}(p_1^{\parallel 2} + p_2^{\parallel 2}) + C_{33}p_3^{\parallel 2} \end{bmatrix} \tag{3.29}$$

$$\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} K_1p_1^{\parallel 2} + (K_1 + K_2 + K_3)p_2^{\parallel 2} + K_4p_3^{\parallel 2} + 2K_5p_1^{\parallel}p_2^{\parallel} & K_5(p_1^{\parallel 2} - p_2^{\parallel 2}) + (K_2 + K_3)p_1^{\parallel}p_2^{\parallel} \\ K_5(p_1^{\parallel 2} - p_2^{\parallel 2}) + (K_2 + K_3)p_1^{\parallel}p_2^{\parallel} & (K_1 + K_2 + K_3)p_1^{\parallel 2} + K_1p_2^{\parallel 2} + K_4p_3^{\parallel 2} - 2K_5p_1^{\parallel}p_2^{\parallel} \end{bmatrix} \tag{3.30}$$

and

$$\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} R_1(p_1^{\parallel 2} - p_2^{\parallel 2}) + 2R_2p_1^{\parallel}p_2^{\parallel} & -R_2(p_1^{\parallel 2} - p_2^{\parallel 2}) + 2R_1p_1^{\parallel}p_2^{\parallel} \\ R_2(p_1^{\parallel 2} - p_2^{\parallel 2}) - 2R_1p_1^{\parallel}p_2^{\parallel} & R_1(p_1^{\parallel 2} - p_2^{\parallel 2}) + 2R_2p_1^{\parallel}p_2^{\parallel} \\ 0 & 0 \end{bmatrix}. \tag{3.31}$$

3.2.2. Laue class 16. The $\mathbf{A}^{\parallel,\parallel}(\boldsymbol{p}^{\parallel})$ block takes the same form as equation (3.29). However, in this case elastic constants K_5 and R_2 vanish compared with Laue class 15. Consequently $\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel})$ and $\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel})$ blocks are

$$\mathbf{A}^{\perp,\perp}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} K_1p_1^{\parallel 2} + (K_1 + K_2 + K_3)p_2^{\parallel 2} + K_4p_3^{\parallel 2} & (K_2 + K_3)p_1^{\parallel}p_2^{\parallel} \\ (K_2 + K_3)p_1^{\parallel}p_2^{\parallel} & (K_1 + K_2 + K_3)p_1^{\parallel 2} + K_1p_2^{\parallel 2} + K_4p_3^{\parallel 2} \end{bmatrix} \tag{3.32}$$

and

$$\mathbf{A}^{\parallel,\perp}(\boldsymbol{p}^{\parallel}) = \begin{bmatrix} R_1(p_1^{\parallel 2} - p_2^{\parallel 2}) & 2R_1 p_1^{\parallel} p_2^{\parallel} \\ -2R_1 p_1^{\parallel} p_2^{\parallel} & R_1(p_1^{\parallel 2} - p_2^{\parallel 2}) \\ 0 & 0 \end{bmatrix}. \tag{3.33}$$

4. Contours of constant diffuse scattering intensity

Using the formulae derived above, we simulated contours of constant diffuse scattering intensity for octagonal quasicrystals. In calculation, we use the ratios of elastic constants because peak shapes are determined by the relative values of elastic constants but not their absolute values. Lattice constants are taken as $a = 7.1$ Å, $c = 6.3$ Å.

Point groups $8/m$ and $8/mmm$ represent symmetries of Laue classes 15 and 16 respectively. Figure 1 represents a plane perpendicular to the periodic direction with quenched phason displacements for the case of Laue class 15. It is assumed that phason quench temperature $T_q = 3\,T$. The diffuse scattering patterns in this plane show eightfold rotation symmetry which is consistent with point group $8/m$.

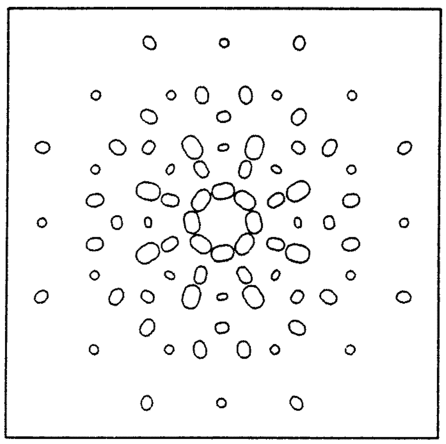

Figure 1. Contours of constant diffuse scattering intensity in a plane perpendicular to the periodic axis with quenched phasons when $T = \frac{1}{3}T_q$ for the case of Laue class 15. Elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = -0.1$, $C_{33}(T) = 0.4$, $C_{44}(T) = 0.6$, $C_{66}(T) = 0.8$, $R_1(T) = 0.05$, $R_2(T) = 0.03$, $C_{11}(T_q) = 0.9$, $C_{13}(T_q) = 0.2$, $C_{33}(T_q) = 0.3$, $C_{44}(T_q) = 0.5$, $C_{66}(T_q) = 0.6$, $R_1(T_q) = 0.04$, $R_2(T_q) = 0.02$, $K_1(T_q) = 0.9$, $K_2(T_q) = -0.2$, $K_3(T_q) = -0.3$, $K_4(T_q) = 0.4$ and $K_5(T_q) = 0.1$.

Figures 2 and 3 give the results for the case of Laue class 16 which we would like to discuss in detail. Figures 2(a) and (b) illustrate diffuse scattering patterns in the plane perpendicular to the periodic direction for quenched phasons corresponding to two sets of different ratios of elastic constants. It it still assumed that $T_q = 3T$. It is obvious that the contour shapes around the same Bragg spots are quite different in figures 2(a) and (b). Figure 2(c) represents the same plane provided that both phonons and phasons are thermalized at T. Therefore, only elastic constants at T are involved in calculation. We take the same values of phonon and phonon–phason coupling elastic constants as those in figure 2(a). Compared with figure 2(a), the diffuse scattering decreased accompanied by slight variation of contour shapes around the

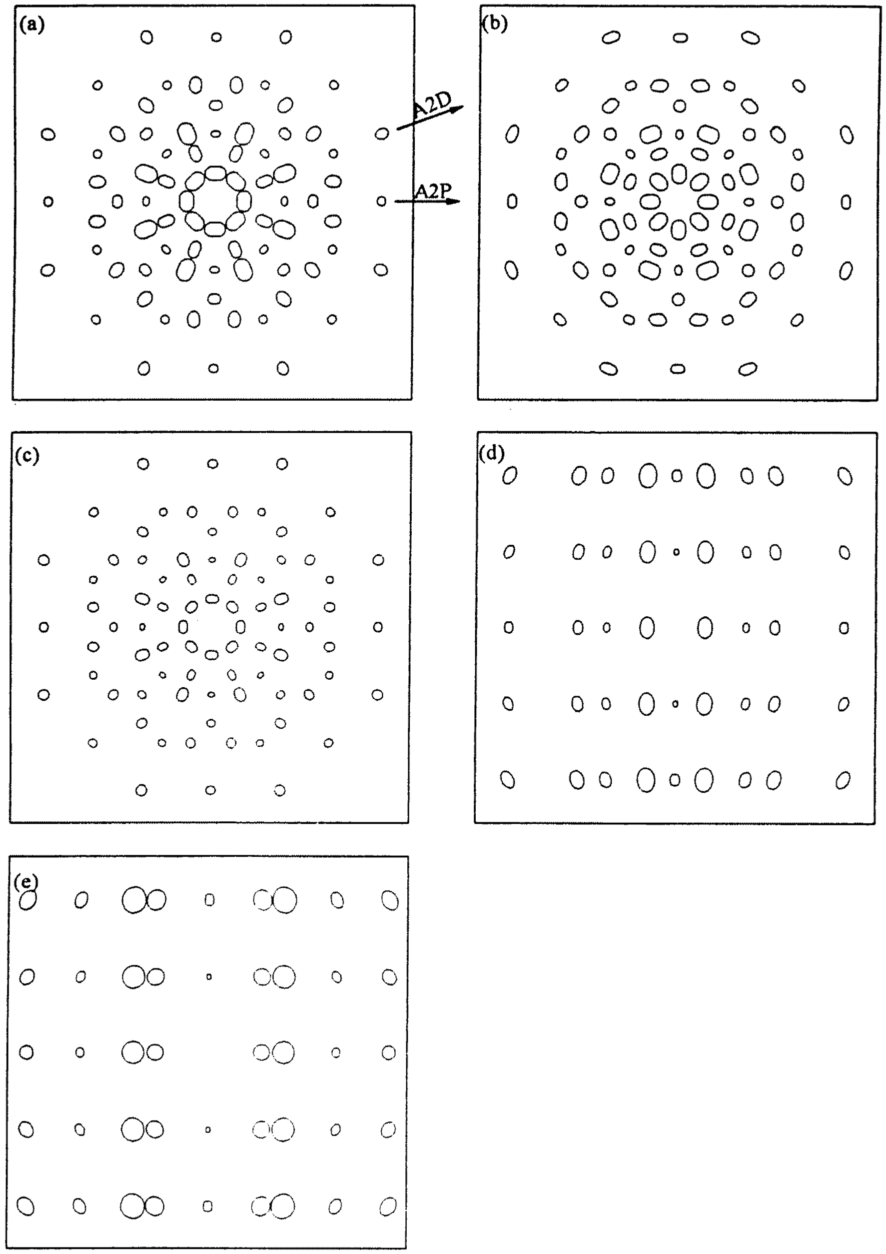

Figure 2. Isointensity contours in planes for the case of Laue class 16. (a), (d) and (e) correspond, respectively, to planes perpendicular to eightfold, A2P and A2D axes with quenched phasons when $T = \frac{1}{3}T_q$. Elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = -0.1$, $C_{33}(T) = 0.4$, $C_{44}(T) = 0.6$, $C_{66}(T) = 0.8$, $R_1(T) = 0.05$, $C_{11}(T_q) = 0.9$, $C_{13}(T_q) = 0.2$, $C_{33}(T_q) = 0.3$, $C_{44}(T_q) = 0.5$, $C_{66}(T_q) = 0.6$, $R_1(T_q) = 0.04$, $K_1(T_q) = 0.9$, $K_2(T_q) = -0.2$, $K_3(T_q) = -0.3$ and $K_4(T_q) = 0.4$. (b) Similar to (a) except that elastic constants are taken as $C_{11}(T) = 1.0$, $C_{13}(T) = 0.2$, $C_{33}(T) = 0.6$, $C_{44}(T) = 0.3$, $C_{66}(T) = 0.4$, $R_1(T) = -0.05$, $C_{11}(T_q) = 0.9$, $C_{13}(T_q) = -0.1$, $C_{33}(T_q) = 0.4$, $C_{44}(T_q) = 0.2$, $C_{66}(T_q) = 0.3$, $R_1(T_q) = -0.08$, $K_1(T_q) = 0.5$, $K_2(T_q) = 0.4$, $K_3(T_q) = 0.2$ and $K_4(T_q) = 0.6$. (c) The same as (a) except that phasons are assumed to be thermalized. Phason elastic constants are taken as $K_1(T) = 0.7$, $K_2(T) = -0.1$, $K_3(T) = -0.2$ and $K_4(T) = 0.5$.

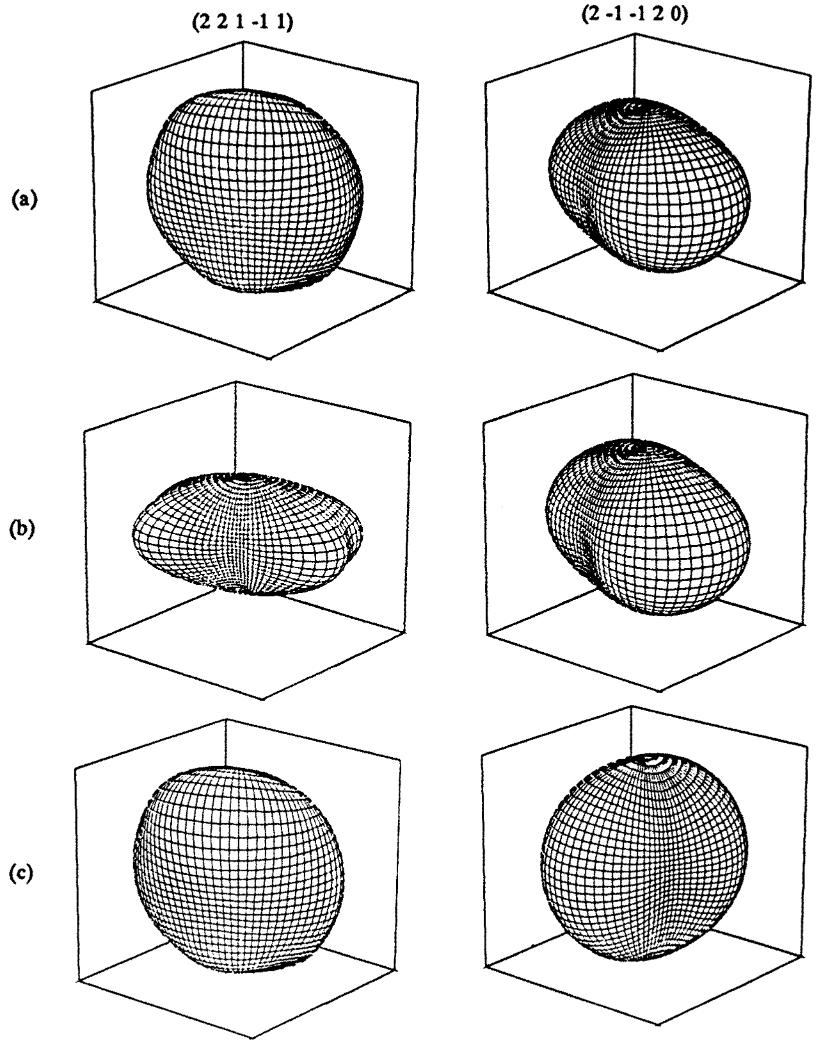

Figure 3. Comparisons of stereoscopic contours around Bragg spots (2 2 1 −1 1) and (2 −1 −1 2 0) with quenched phasons when $T = \frac{1}{3}T_q$ for the case of Laue class 16. Phonon–phason coupling elastic constants are taken as $R_1(T) = -0.1$ and $R_1(T_q) = -0.05$. The other parameters are taken as follows: (a) $C_{11}(T) = 1.0$, $C_{13}(T) = 0.2$, $C_{33}(T) = 0.5$, $C_{44}(T) = 0.6$, $C_{56}(T) = 0.7$, $C_{11}(T_q) = 0.9$, $C_{13}(T_q) = 0.1$, $C_{33}(T_q) = 0.4$, $C_{44}(T_q) = 0.5$, $C_{66}(T_q) = 0.6$, $K_1(T_q) = 0.9$, $K_2(T_q) = -0.2$, $K_3(T_q) = -0.4$ and $K_4(T_q) = 0.7$; (b) $C_{11}(T) = 1.0$, $C_{13}(T) = -0.3$, $C_{33}(T) = 0.3$, $C_{44}(T) = 0.5$, $C_{66}(T) = 0.2$, $C_{11}(T_q) = 0.9$, $C_{13}(T_q) = -0.2$, $C_{33}(T_q) = 0.2$, $C_{44}(T_q) = 0.6$, $C_{66}(T_q) = 0.3$ and the same phason elastic constants as those in (a); (c) the same phonon elastic constants as those in (a) and $K_1(T_q) = 0.6$, $K_2(T_q) = 0.8$, $K_3(T_q) = 0.7$, $K_4(T_q) = 0.6$.

same Bragg spots due to the reduced contribution of phason disorder. If the diffuse scattering patterns like those in figures 2(a)–(c) could be detected and measured precisely, one could use these patterns to extract information about elastic constants. Such experiments have been done on a single grain of Al–Pd–Mn icosahedral phase using elastic neutron scattering (de Boissieu *et al* 1995, Boudard *et al* 1996). It follows from equations (3.29) and (3.32) that terms containing elastic constants C_{13}, C_{33} and K_4 vanish in matrix $\mathbf{A}(\boldsymbol{p}^{\parallel})$ if the diffuse scattering patterns are measured in the plane perpendicular to the periodic direction as in figures 2(a)–(c) so that such patterns are insufficient to acquire all of the elastic constants. Figures 2(d) and (e) show patterns perpendicular, respectively, to twofold axes A2P, which is along the direction of arbitrary basis vector in quasiperiodic plane or its equivalent direction, and A2D, which is along a bisector between any of these basis vectors and its neighbouring equivalent direction with the same conditions as for figure 2(a), and they may be used to give information about the other elastic constants that figures 2(a)–(c) cannot present.

The symmetries of diffuse scattering patterns shown in figure 2 are consistent with point group $8/mmm$. There are two kinds of mirror in figures 2(a)–(c) besides an eightfold rotation axis along the periodic direction. One is perpendicular to A2P and the other perpendicular to A2D.

As shown in the figures above, in comparison with ordinary crystals, anisotropic contour shapes of quasicrystals are much more complicated and the contour shapes vary from spot to spot, even for collinear Bragg spots.

Figure 3 presents comparison of stereoscopic contours of constant diffuse scattering intensity around Bragg spots $(2\,2\,1\,{-1}\,1)$ and $(2\,{-1}\,{-1}\,2\,0)$ for quenched phasons when $T = \frac{1}{3}T_q$. In the calculations, we consider three sets of elastic constants. Only phonon elastic constants in figure 3(b) and phason elastic constants in figure 3(c) are changed with respect to those in figure 3(a). It is evident that the shape of isointensity contour around reflection $(2\,{-1}\,{-1}\,2\,0)$ which has a large $\boldsymbol{Q}^{\perp}$ component varies greatly in figure 3(c) but slightly in figure 3(b) in comparison with that in figure 3(a) while exactly the reverse results can be found for reflection $(2\,2\,1\,{-1}\,1)$ which has a large $\boldsymbol{Q}^{\parallel}$ component. The fact that peak shapes of Bragg spots with large $\boldsymbol{Q}^{\perp}$ component are dominated by phason elastic constants can be accounted for by special phason degrees of freedom in quasicrystals which also give rise to the variation of peak shapes among collinear Bragg spots.

In summary general formulae for thermal diffuse scattering from quasicrystals are applied to the case of octagonal quasicrystals from corresponding elasticity theory. Contours of constant diffuse scattering intensity were calculated to examine the effect of phonon and phason disorders on diffuse scattering from octagonal quasicrystals. The symmetries of diffuse scattering patterns are consistent with corresponding point groups. Unlike ordinary crystals, shapes of isointensity contours are much more complicated and vary even among the collinear Bragg spots due to the additional phason degrees of freedom. Information about elastic constants can be extracted from quantitative analysis of diffuse scattering patterns.

Acknowledgment

This work was supported by the National Natural Science Foundation of China.

Appendix. Coordinate systems for octagonal quasicrystals

Structural descriptions of octagonal quasicrystals are conveniently done in a 5D embedding space $E = (E^{\parallel}, E^{\perp})$ which consists of two orthogonal subspaces, the 3D physical or parallel space $E^{\parallel}$ with orthogonal unit basis vectors $\boldsymbol{E}_1^{\parallel}$, $\boldsymbol{E}_2^{\parallel}$, $\boldsymbol{E}_3^{\parallel}$ and 2D complementary or perpendicular space $E^{\perp}$ with orthogonal unit basis vectors $\boldsymbol{E}_1^{\perp}$, $\boldsymbol{E}_2^{\perp}$. The diffraction pattern of octagonal quasicrystals may be indexed using the combination of five reciprocal basis vectors

e_i^*, $i = 1, 2, \ldots, 5$, which can be written as

$$\begin{bmatrix} e_1^* \\ e_2^* \\ e_3^* \\ e_4^* \\ e_5^* \end{bmatrix} = a^* \begin{bmatrix} \cos\left(\frac{0\pi}{4}\right) & \sin\left(\frac{0\pi}{4}\right) & 0 & \cos\left(\frac{0\pi}{4}\right) & \sin\left(\frac{0\pi}{4}\right) \\ \cos\left(\frac{1\pi}{4}\right) & \sin\left(\frac{1\pi}{4}\right) & 0 & \cos\left(\frac{3\pi}{4}\right) & \sin\left(\frac{3\pi}{4}\right) \\ \cos\left(\frac{2\pi}{4}\right) & \sin\left(\frac{2\pi}{4}\right) & 0 & \cos\left(\frac{6\pi}{4}\right) & \sin\left(\frac{6\pi}{4}\right) \\ \cos\left(\frac{3\pi}{4}\right) & \sin\left(\frac{3\pi}{4}\right) & 0 & \cos\left(\frac{9\pi}{4}\right) & \sin\left(\frac{9\pi}{4}\right) \\ 0 & 0 & \frac{c^*}{a^*} & 0 & 0 \end{bmatrix} \begin{bmatrix} E_1^{\parallel} \\ E_2^{\parallel} \\ E_3^{\parallel} \\ E_1^{\perp} \\ E_2^{\perp} \end{bmatrix}$$

$$= a^* \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 0 & 1 & 0 & 0 & -1 \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 0 & 0 & \frac{c^*}{a^*} & 0 & 0 \end{bmatrix} \begin{bmatrix} E_1^{\parallel} \\ E_2^{\parallel} \\ E_3^{\parallel} \\ E_1^{\perp} \\ E_2^{\perp} \end{bmatrix} \qquad \text{(A.1)}$$

where a^* and c^* are the reciprocal lattice constants. The direct basis vectors e_i, $i = 1, 2, \ldots, 5$, in 5D embedding space are given by

$$\begin{bmatrix} e_1^{\parallel} \\ e_2^{\parallel} \\ e_3^{\parallel} \\ e_4^{\parallel} \\ e_5^{\parallel} \end{bmatrix} = \frac{a}{2} \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 0 & 1 & 0 & 0 & -1 \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 0 & 0 & \frac{2c}{a} & 0 & 0 \end{bmatrix} \begin{bmatrix} E_1^{\parallel} \\ E_2^{\parallel} \\ E_3^{\parallel} \\ E_1^{\perp} \\ E_2^{\perp} \end{bmatrix} \qquad \text{(A.2)}$$

where a, c are the lattice constants and $a = 1/a^*$, $c = 1/c^*$.

References

Bak P 1985a *Phys. Rev. Lett.* **54** 1517
——1985b *Phys. Rev.* B **32** 5764
Bancel P A and Heiney P 1986 *J. Physique Coll.* **47** C3 341
Bancel P A, Heiney P A, Stephens P W, Goldman A E and Horn P M 1985 *Phys. Rev. Lett.* **54** 2422
Boudard M, de Boissieu M, Letoublon A, Hennion B, Bellissent B and Janot C 1996 *Europhys. Lett.* **33** 199
Cao W, Ye H Q and Kuo K H 1988 *Phys. Status Solidi* a **107** 511
de Boissieu M, Boundard M, Hennion B, Belissent R, Kycia S, Goldman A, Janot C and Audier M 1995 *Phys. Rev. Lett.* **75** 89
Ding D H, Yang W G, Hu C Z and Wang R 1993 *Phys. Rev.* B **48** 7003
Horn P M, Malzfeldt W, Di Vincenzo D P, Toner J and Gambino R 1986 *Phys. Rev. Lett.* **57** 1444
Hu C Z, Ding D H and Yang W G 1993 *Acta. Phys. Sin.* **2** 42
Hu C Z, Wang R, Yang W G and Ding D H 1996 *Acta Crystallogr.* A **52** 521
Hu C Z, Yang W G, Wang R and Ding D H 1997 *Prog. Phys.* **17** 345 (in Chinese)
Ishii Y 1992 *Phys. Rev.* B **45** 5228
Janssen T 1992 *Z. Kristallogr.* **198** 17

Jaric M V and Nelson D R 1988 *Phys. Rev.* B **37** 4458
Jennings A 1977 *Matrix Computation for Engineers and Scientists* (London: Wiley)
Lei J L, Wang R, Hu C Z and Ding D H 1999 *Phys. Rev.* B **59**
Levine D, Lubensky T C, Ostlund S, Ramaswamy S, Steinhardt P J and Toner J 1985 *Phys. Rev. Lett.* **54** 1520
Lubensky T C, Ramaswamy S and Toner J 1985 *Phys. Rev.* B **32** 7444
Lubensky T C, Socolar J E S, Steinhardt P J, Bancel P A and Heiney P A 1986 *Phys. Rev. Lett.* **57** 1440
Shechtman D, Blech I, Gratias D and Cahn J W 1984 *Phys. Rev. Lett.* **53** 1951
Socolar J E S 1989 *Phys. Rev.* B **39** 10 519
Socolar J E S and Wright D C 1987 *Phys. Rev. Lett.* **59** 211
Wang N, Chen H and Kuo K H 1987 *Phys. Rev. Lett.* **59** 1010
Wang N, Fung K K and Kuo K H 1988 *Appl. Phys. Lett.* **52** 2120
Wang Z M and Kuo K H 1988 *Acta Crystallogr.* A **44** 857
Widom M 1991 *Phil. Mag. Lett.* **64** 297
Wooster W A 1962 *Diffuse X-ray Reflections from Crystals* (Oxford: Clarendon)
Yang W G, Wang R, Ding D H and Hu C Z 1995 *J. Phys.: Condens. Matter* **7** 7099