Diffuse scattering from decagonal quasicrystals

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(Received 21 April 1998)

General formulas for both thermal and quenched diffuse scattering from quasicrystals are applied to the case of decagonal quasicrystals from corresponding elasticity theory. Contours of constant diffuse scattering intensity are illustrated. 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. Quantitative examination of diffuse scattering patterns may yield numerical values of the elastic constants. [S0163-1829(99)01901-3]

I. INTRODUCTION

Since the discovery of the icosahedral quasicrystals in Al-Mn alloys,[1] several quasicrystals, such as the decagonal,[2] dodecagonal,[3] and octagonal phases[4] have been reported. Atomic structure and physical properties of such materials have been the focus of many theoretical and experimental works especially since the discoveries of stable icosahedral phases in Al-Cu-Fe (Ref. 5) and Al-Pd-Mn (Ref. 6) systems and decagonal phase in Al-Cu-Co (Ref. 7) system. 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.[8,9] How strains in phonon and phason variables or quenched dislocations can lead to these experimental observations has been discussed.[10,11] Furthermore, although the Al-Pd-Mn icosahedral phase displays very good long-range quasiperiodic order, it was shown that some diffuse scattering is located close to the Bragg reflections.[12] Socolar and Wright have examined the shapes of Bragg spots observed in icosahedral phases and reproduced the peak shapes by the superposition of uniform phason strains.[13] Elastic property of icosahedral quasicrystals has been the object of many theoretical works.[14–17] Jaric and Nelson 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.[18] With the help of this theory, the onset of hydrodynamic instability of icosahedral phases has been discussed;[19,20] 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.[21,22]

Decagonal quasicrystals represent interesting immediate states between icosahedral and crystalline phases with anisotropic physical and mechanical properties. The stable decagonal phases have been synthesized in many alloy systems. Elasticity of planar quasicrystals with tenfold symmetry has been discussed in some papers.[23,24] Some investigators have restricted attention to two-dimensional (2D) quasicrystals including decagonal quasicrystals.[25–27] Based on the 5D crystallographic symmetry operations listed by Janssen,[28] they have derived all possible point groups of 2D quasicrystals of rank 5 and calculated the numbers of independent forth-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.

In this paper, we would like to discuss diffuse scattering from decagonal quasicrystals theoretically. Point groups, Laue classes, and elastic properties of decagonal quasicrystals are summarized in Sec. II. Diffuse scattering from decagonal quasicrystals is formulated in Sec. III. Contours of constant diffuse scattering intensity are illustrated and analysis of the results are given in Sec. IV.

II. POINT GROUPS, LAUE CLASSES, AND ELASTIC PROPERTIES OF DECAGONAL SYSTEM

In this section we will illustrate the determination of explicit forms of invariant terms in the elastic energy and elastic constant tensor for decagonal 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.[24,25,27]

If an analytic expression of the elastic free energy is possible, it will be quadratic in the special gradients of phonon displacements $\mathbf{u}^{\parallel}$ and phason displacements $\mathbf{u}^{\perp}$ 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 must 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 10mm (D_{10}) generated by a tenfold rotation α and a mirror β, which can be represented by

$$\Gamma(\alpha)=\begin{bmatrix} 0 & 0 & 0 & -1 & 0\\ 1 & 1 & 1 & 1 & 0\\ -1 & 0 & 0 & 0 & 0\\ 0 & -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

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

The coordinate systems which we use for decagonal quasicrystals are the same as those described in Refs. 29 and 30. The matrix representation Γ reduces to

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

It follows that $\mathbf{u}^{\parallel}$ transforms under $\Gamma_5+\Gamma_1$ and $\mathbf{u}^{\perp}$ transforms under Γ_7. Therefore, the displacement gradients $\partial_j u_i^{\parallel}$ $(i,j=1,2,3)$ 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 $\mathbf{u}^{\parallel}$ is a three-component vector while $\mathbf{u}^{\perp}$ 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 $\partial_j u_i^{\parallel}$ 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:

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

where $E_{ij}=\frac{1}{2}(\partial_j u_i^{\parallel}+\partial_i u_j^{\parallel})$ 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

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

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

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

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

$$(\Gamma_5+\Gamma_1)\times\Gamma_7=\Gamma_6+\Gamma_8+\Gamma_7. \tag{2.7}$$

Three pairs $(\partial_1 u_1^{\perp}+\partial_2 u_2^{\perp},\ \partial_1 u_2^{\perp}-\partial_2 u_1^{\perp})$, $(\partial_1 u_1^{\perp}-\partial_2 u_2^{\perp},\ \partial_1 u_2^{\perp}+\partial_2 u_1^{\perp})$ and $(\partial_3 u_1^{\perp},\ \partial_3 u_2^{\perp})$ span three different representations Γ_6, Γ_8, and Γ_7, respectively. Thus we can obtain three quadratic invariants

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

$$(\partial_1 u_1^{\perp}-\partial_2 u_2^{\perp})^2+(\partial_1 u_2^{\perp}+\partial_2 u_1^{\perp})^2, \quad (\partial_3 u_1^{\perp})^2+(\partial_3 u_2^{\perp})^2. \tag{2.8}$$

and three independent elastic constants. Nonvanishing elastic constants are

$$K_{1111}=K_{2222}=K_{1212}=K_{2121}=K_1,$$

$$K_{1122}=K_{2211}=-K_{1221}=-K_{2112}=K_2, \quad K_{1313}=K_{2323}=K_4. \tag{2.9}$$

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

$$(E_{11}-E_{22})(\partial_1 u_1^{\perp}+\partial_2 u_2^{\perp})+2E_{12}(\partial_1 u_2^{\perp}-\partial_2 u_1^{\perp}) \tag{2.10}$$

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

$$R_{1111}=R_{1122}=-R_{2211}=-R_{2222}=R_{1221}$$
$$=R_{2121}=-R_{1212}=-R_{2112}=R_1. \tag{2.11}$$

Therefore, it can be seen that there are nine quadratic invariants and hence nine independent elastic constants for 10mm. Among them five elastic constants are associated with the phonon field, three 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 10 (C_{10}) symmetry. There are ten quadratic invariants and hence ten independent elastic constants. Among them nine elastic constants are the same as those for 10mm; another nonvanishing phonon-phason coupling elastic constant is

$$R_{1112}=-R_{1121}=-R_{2212}=R_{2221}=R_{1211}$$
$$=R_{2111}=R_{1222}=R_{2122}=R_2. \tag{2.12}$$

Decagonal system has seven point groups divided into two Laue classes which we term Laue classes 13 and 14, respectively. Laue class 13 includes 10, $\overline{10}$, 10/m while Laue class 14 includes 10mm, 1022, $\overline{10}$m2, 10/mmm. Elastic properties possess an inherent centrosymmetry. Therefore, all point groups belonging to the same Laue class possess the same elastic properties.

III. FORMULAS FOR DIFFUSE SCATTERING FROM DECAGONAL QUASICRYSTALS

Following the method given by Jaric and Nelson,[18] and Ishii,[20] we will present the generalized theory of diffuse scattering from quasicrystals within the framework of the hydrodynamic theory. The formulas derived here are modifications of those originally put forward by Jaric and Nelson.[18] Such modified formulas have a clear advantage, i.e., the formulas appropriate for the case of quenched phasons can be automatically evolved into those appropriate for the case of thermal phasons. Moreover, the expressions here are not limited to simple quasilattice[18] and may be used for any quasicrystals.

The structure of quasilattice can be constructed by cutting a d-dimensional crystal. The density of a perfect quasilattice can be represented by

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

where $\parallel$ and $\perp$ denote the physical and complementary subspaces, respectively; ρ is a periodic density in the hyperspace. Explicitly,

$$\rho(\mathbf{x})=\sum_{\mathbf{R}}\delta(\mathbf{x}-\mathbf{R})*\rho_c(\mathbf{x}), \tag{3.2}$$

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

$$\Phi(\mathbf{q})=\int \rho(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}d^dx=\sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}}F(\mathbf{q})$$
$$=\frac{(2\pi)^d}{\nu_c}\sum_{\mathbf{Q}}\delta(\mathbf{q}-\mathbf{Q})F(\mathbf{Q}), \tag{3.3}$$

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

$$F(\mathbf{q})=\int \rho_c(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}d^dx \tag{3.4}$$

is the structure factor of unit hypercell. Since the Fourier transform of a cut is equal to a projection of a Fourier transform, the scattering amplitude of a perfect quasicrystal can be given by

$$\Phi^{\parallel}(\mathbf{q}^{\parallel})=\int \Phi(\mathbf{q})d^{d-3}q^{\perp}=\frac{(2\pi)^d}{\nu_c}\sum_{\mathbf{Q}}\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{Q}^{\parallel})F(\mathbf{Q}). \tag{3.5}$$

It can also be written in the form

$$\Phi^{\parallel}(\mathbf{q}^{\parallel})=\int \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}}F(\mathbf{k})\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{k}^{\parallel})d^dk \tag{3.6}$$

which facilitates extending to the case of disordered quasicrystals.

The elastic free energy of a disordered quasicrystal of volume V can be written in terms of the Fourier transform $\mathbf{u}(\mathbf{p}^{\parallel})$ of displacements $\mathbf{u}$,

$$E=\frac{(2\pi)^3}{2}\int \mathbf{u}(-\mathbf{p}^{\parallel})\cdot(\mathbf{p}^{\parallel}\cdot\mathbf{M}\cdot\mathbf{p}^{\parallel})\cdot\mathbf{u}(\mathbf{p}^{\parallel})d^3p^{\parallel}, \tag{3.7}$$

or in terms of phonon, phason and phonon-phason coupling contributions,

$$E=E_{\text{phon}}[\mathbf{u}^{\parallel}]+E_{\text{phas}}[\mathbf{u}^{\perp}]+E_{\text{coup}}[\mathbf{u}^{\parallel},\mathbf{u}^{\perp}], \tag{3.8}$$

where $\mathbf{M}$ is the elastic modulus tensor.

If the unit hypercell is displaced by a vector $\mathbf{u}(\mathbf{R}^{\parallel})$ from its proper position $\mathbf{R}$, then Eq. (3.6) should be replaced by

$$\Phi^{\parallel}(\mathbf{q}^{\parallel})=\int \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot[\mathbf{R}+\mathbf{u}(\mathbf{R}^{\parallel})]}F(\mathbf{k})\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{k}^{\parallel})d^dk. \tag{3.9}$$

The scattering intensity must be averaged over a distribution $P[\mathbf{u}]$ of $\mathbf{u}$. Therefore, it can be written as

$$I(\mathbf{q}^{\parallel})=|\Phi^{\parallel}(\mathbf{q}^{\parallel})|^2$$
$$=\sum_{\mathbf{R}_1\mathbf{R}_2}\int\int e^{i\mathbf{k}_2\cdot\mathbf{R}_2-i\mathbf{k}_1\cdot\mathbf{R}_1}fF(\mathbf{k}_1)$$
$$\times F^*(\mathbf{k}_2)\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{k}_1^{\parallel})\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{k}_2^{\parallel})d^dk_1d^dk_2, \tag{3.10}$$

where f denotes the average

$$f=\int \mathcal{D}(\mathbf{u})e^{i\mathbf{k}_2\cdot\mathbf{u}(\mathbf{R}_2^{\parallel})-i\mathbf{k}_1\cdot\mathbf{u}(\mathbf{R}_1^{\parallel})}P[\mathbf{u}]. \tag{3.11}$$

$P[\mathbf{u}]$ is a Boltzmann distribution associated with the elastic energy given by Eq. (3.7),

$$P[\mathbf{u}]\propto\exp\left[-\frac{(2\pi)^3}{2k_BT}\int \mathbf{u}(-\mathbf{p}^{\parallel})\cdot(\mathbf{p}^{\parallel}\cdot\mathbf{M}\cdot\mathbf{p}^{\parallel})\cdot\mathbf{u}(\mathbf{p}^{\parallel})d^3p^{\parallel}\right], \tag{3.12}$$

where T is temperature and k_B is the Boltzmann constant.

Following the derivation given by Jaric and Nelson,[18] the scattering intensity can be written as an expansion

$$I(\mathbf{q}^{\parallel})=I_0(\mathbf{q}^{\parallel})+I_1(\mathbf{q}^{\parallel})+\cdots, \tag{3.13}$$

whose first two terms are the Bragg scattering

$$I_0(\mathbf{q}^{\parallel})=\frac{V}{(2\pi)^3}\frac{(2\pi)^{2d}}{\nu_c^2}\sum_{\mathbf{Q}}\delta^{\parallel}(\mathbf{q}^{\parallel}-\mathbf{Q}^{\parallel})|F(\mathbf{Q})|^2e^{-2W(\mathbf{Q})}, \tag{3.14}$$

and the lowest-order diffuse scattering

$$I_1(\mathbf{q}^{\parallel})=\frac{Vk_BT}{(2\pi)^6}\frac{(2\pi)^{2d}}{\nu_c^2}\sum_{\mathbf{Q}}(\mathbf{q}^{\parallel}\mathbf{Q}^{\perp})\cdot\mathbf{A}^{-1}(\mathbf{q}^{\parallel}-\mathbf{Q}^{\parallel})\cdot\begin{pmatrix}\mathbf{q}^{\parallel}\\ \mathbf{Q}^{\perp}\end{pmatrix}$$
$$\times|F(\mathbf{q}^{\parallel},\mathbf{Q}^{\perp})|^2e^{-2W(\mathbf{q}^{\parallel},\mathbf{Q}^{\perp})}, \tag{3.15}$$

where

$$e^{-2W(\mathbf{q})}=\exp\left[-\frac{k_BT}{(2\pi)^3}\int \mathbf{q}\cdot\mathbf{A}^{-1}(\mathbf{p}^{\parallel})\cdot\mathbf{q}d^3p^{\parallel}\right] \tag{3.16}$$

is the Debye-Waller factor.

Near a particular Bragg spot $\mathbf{Q}$ the scattering intensity can be written as

$$I(\mathbf{Q}^{\parallel}+\mathbf{p}^{\parallel})\approx\frac{V}{(2\pi)^3}\frac{(2\pi)^{2d}}{\nu_c^2}|F(\mathbf{Q})|^2$$
$$\times e^{-2W(\mathbf{Q})}\left[\delta^{\parallel}(\mathbf{p}^{\parallel})+\frac{k_BT}{(2\pi)^3}\mathbf{Q}\cdot\mathbf{A}^{-1}(\mathbf{p}^{\parallel})\cdot\mathbf{Q}\right]. \tag{3.17}$$

The hydrodynamic matrix $\mathbf{A}(\mathbf{p}^{\parallel})$ is related to the elastic modulus tensor $\mathbf{M}$ of the quasicrystal. If the temperature is high enough, then phasons, as well as phonons, are thermalized; the matrix $\mathbf{A}(\mathbf{p}^{\parallel})$ can be given by

$$A_{\mu,\nu}(\mathbf{p}^{\parallel})=p_j^{\parallel}M_{\mu,j;\nu,l}p_l^{\parallel}. \tag{3.18}$$

Obviously, it can be divided into four blocks $\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})$, $\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})$, $\mathbf{A}^{\perp,\parallel}(\mathbf{p}^{\parallel})$ and $\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})$:

$$[\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})]_{ik}=p_j^{\parallel}C_{ijkl}p_l^{\parallel}, \tag{3.19}$$

$$[\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})]_{ik}=p_j^{\parallel}K_{ijkl}p_l^{\parallel}, \tag{3.20}$$

and

$$[\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})]_{ik}=[\mathbf{A}^{\perp,\parallel}(\mathbf{p}^{\parallel})]_{ki}=p_j^{\parallel}R_{ijkl}p_l^{\parallel}. \tag{3.21}$$

If 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 $\mathbf{u}_q^{\perp}$. Therefore, the average in Eq. (3.11) will require two steps. The first step is the same as described by Jaric and Nelson.[18] The second step is associated with $\mathbf{u}_q^{\perp}$. Since there exists coupling between $\mathbf{u}_q^{\parallel}$ and $\mathbf{u}_q^{\perp}$ at T_q, the ensemble average must be averaged over $\mathbf{u}_q$ using the Boltzmann distribution $P_q[\mathbf{u}_q]$,

$$P_q[\mathbf{u}_q]\propto \exp\left[-\frac{E_q}{k_BT_q}\right], \tag{3.22}$$

where elastic free energy at T_q is

$$E_q=E_{\text{phon}}[\mathbf{u}_q^{\parallel}]+E_{\text{phas}}[\mathbf{u}_q^{\perp}]+E_{\text{coup}}[\mathbf{u}_q^{\parallel},\mathbf{u}_q^{\perp}]. \tag{3.23}$$

It can be verified that $\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})$, $\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})$, and $\mathbf{A}^{\perp,\parallel}(\mathbf{p}^{\parallel})$ blocks can still be given by Eqs. (3.19) and (3.21) but $\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})$ block should be modified by

$$\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})=\frac{T}{T_q}\{\mathbf{A}_q^{\perp,\perp}(\mathbf{p}^{\parallel})-\mathbf{A}_q^{\perp,\parallel}(\mathbf{p}^{\parallel})\cdot[\mathbf{A}_q^{\parallel,\parallel}(\mathbf{p}^{\parallel})]^{-1}\cdot\mathbf{A}_q^{\parallel,\perp}(\mathbf{p}^{\parallel})\}+\mathbf{A}^{\perp,\parallel}(\mathbf{p}^{\parallel})\cdot[\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})]^{-1}\cdot\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel}), \tag{3.24}$$

where the subscript q means that the values of the elastic constants at T_q should be used. It should be emphasized that matrix $\mathbf{A}(\mathbf{p}^{\parallel})$ is associated not only with phonon and phonon-phason 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, Eq. (3.24) will be reduced to Eq. (3.20) if $T=T_q$, which is physically reasonable.

It has been pointed out in Sec. II 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 $\mathbf{A}(\mathbf{p}^{\parallel})$ is identical for all point groups belonging to the same Laue class. From elastic properties of decagonal quasicrystals, explicit expressions of $\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})$, $\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})$, and $\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})$ blocks for each Laue class of decagonal system can be easily obtained.

For Laue class 13, $\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})$, $\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})$, and $\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})$ blocks are given by

$$\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})=\begin{bmatrix} C_{11}p_1^{\parallel 2}+C_{66}p_2^{\parallel 2}+C_{44}p_3^{\parallel 2} & (C_{11}-C_{66})p_1^{\parallel}p_2^{\parallel} & (C_{44}+C_{13})p_1^{\parallel}p_3^{\parallel} \\ (C_{11}-C_{66})p_1^{\parallel}p_2^{\parallel} & C_{66}p_1^{\parallel 2}+C_{11}p_2^{\parallel 2}+C_{44}p_3^{\parallel 2} & (C_{44}+C_{13})p_2^{\parallel}p_3^{\parallel} \\ (C_{44}+C_{13})p_1^{\parallel}p_3^{\parallel} & (C_{44}+C_{13})p_2^{\parallel}p_3^{\parallel} & C_{44}(p_1^{\parallel 2}+p_2^{\parallel 2})+C_{33}p_3^{\parallel 2} \end{bmatrix}, \tag{3.25}$$

$$\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})=\begin{bmatrix} K_1(p_1^{\parallel 2}+p_2^{\parallel 2})+K_4p_3^{\parallel 2} & 0 \\ 0 & K_1(p_1^{\parallel 2}+p_2^{\parallel 2})+K_4p_3^{\parallel 2} \end{bmatrix}, \tag{3.26}$$

and

$$\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})=\begin{bmatrix} R_1(p_1^{\parallel 2}-p_2^{\parallel 2})+2R_2p_1^{\parallel}p_2^{\parallel} & -R_2(p_1^{\parallel 2}-p_2^{\parallel 2})+2R_1p_1^{\parallel}p_2^{\parallel} \\ R_2(p_1^{\parallel 2}-p_2^{\parallel 2})-2R_1p_1^{\parallel}p_2^{\parallel} & R_1(p_1^{\parallel 2}-p_2^{\parallel 2})+2R_2p_1^{\parallel}p_2^{\parallel} \\ 0 & 0 \end{bmatrix}. \tag{3.27}$$

For Laue class 14, $\mathbf{A}^{\parallel,\parallel}(\mathbf{p}^{\parallel})$ and $\mathbf{A}^{\perp,\perp}(\mathbf{p}^{\parallel})$ blocks take the same forms as Eqs. (3.25) and (3.26), respectively. However, in this case elastic constant R_2 vanishes compared with Laue class 13. Consequently $\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})$ block is

$$\mathbf{A}^{\parallel,\perp}(\mathbf{p}^{\parallel})=\begin{bmatrix} R_1(p_1^{\parallel 2}-p_2^{\parallel 2}) & 2R_1p_1^{\parallel}p_2^{\parallel} \\ -2R_1p_1^{\parallel}p_2^{\parallel} & R_1(p_1^{\parallel 2}-p_2^{\parallel 2}) \\ 0 & 0 \end{bmatrix}. \tag{3.28}$$

IV. CONTOURS OF CONSTANT DIFFUSE SCATTERING INTENSITY

Using the formulas derived above, we calculated contours of constant diffuse scattering intensity for decagonal quasicrystals. In calculation, we use the ratios of elastic constants because peak shapes are determined by the relative values of elastic constants but not the absolute values of them. Lattice constants are taken as $a_i=3.7$ Å, $i=1,2,...,4$ and $a_5=4.5$ Å.

Point groups 10/m, 10/mmm represent symmetries of Laue classes 13 and 14, respectively. Figure 1 represents a plane perpendicular to the periodic direction with quenched phason displacements for the case of Laue class 13. It is assumed that phason quench temperature $T_q=3T$. The diffuse scattering patterns in this plane show tenfold rotation symmetry which is consistent with point group 10/m.

Figures 2 and 3 give the results for the case of Laue class 14 which we would like to discuss in detail. Figures 2(a) and 2(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 is still assumed that $T_q=3T$. It is obvious that the contour shapes around the same Bragg spots are quite different in

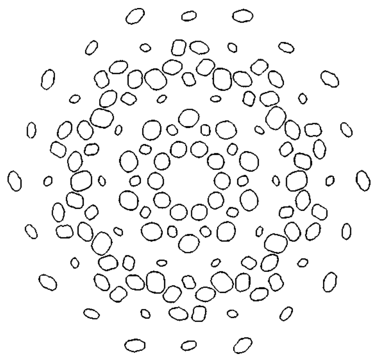

FIG. 1. Contours of constant diffuse scattering intensity in a plane perpendicular to the periodic axis with quenched phasons when $T=\frac{1}{3}T_q$ for the case of Laue class 13. Elastic constants are taken as $C_{11}(T)=1.0$, $C_{13}(T)=-0.1$, $C_{33}(T)=0.3$, $C_{44}(T)=0.2$, $C_{66}(T)=0.4$, $R_1(T)=0.1$, $R_2(T)=0.15$, $C_{11}(T_q)=0.9$, $C_{13}(T_q)=-0.2$, $C_{33}(T_q)=0.2$, $C_{44}(T_q)=0.2$, $C_{66}(T_q)=0.5$, $R_1(T_q)=0.12$, $R_2(T_q)=0.1$, $K_1(T_q)=0.9$, and $K_4(T_q)=0.6$.

Figs. 2(a) and 2(b). Figure 2(c) represents the same plane provided that 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 Fig. 2(a). Compared with Fig. 2(a), the diffuse scattering decreased accompanied by slight variation of contour shapes around the same Bragg spots due to the reduced contribution of phason disorder. If the diffuse scattering patterns like those in Figs. 2(a)–2(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.[21,22] It should be noted that information about elastic constant K_2 cannot be inferred from any diffuse scattering pattern because K_2 does not appear in matrix $\mathbf{A}(\mathbf{p}^{\parallel})$. It follows from Eqs. (3.25) and (3.26) that terms containing elastic constants C_{13}, C_{33}, and K_4 vanish in matrix $\mathbf{A}(\mathbf{p}^{\parallel})$ if the diffuse scattering patterns are

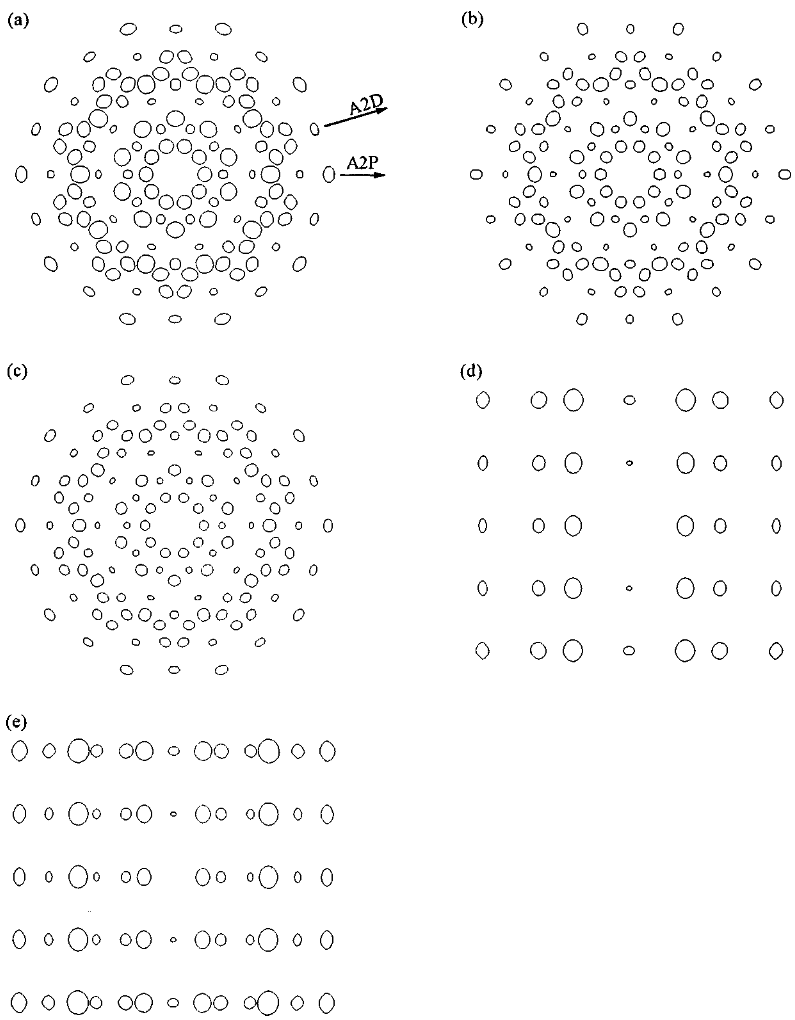

FIG. 2. Isointensity contours in planes for the case of Laue class 14. (a), (d), and (e) correspond, respectively, to planes perpendicular to tenfold, A2P, and A2D axes with quenched phasons when $T=\frac{1}{3}T_q$. Elastic constants are taken as $C_{11}(T)=1.0$, $C_{13}(T)=-0.1$, $C_{33}(T)=0.3$, $C_{44}(T)=0.2$, $C_{66}(T)=0.4$, $R_1(T)=0.1$, $C_{11}(T_q)=0.9$, $C_{13}(T_q)=-0.2$, $C_{33}(T_q)=0.2$, $C_{44}(T_q)=0.2$, $C_{66}(T_q)=0.5$, $R_1(T_q)=0.12$, $K_1(T_q)=0.9$, and $K_4(T_q)=0.6$. (b) Similar to (a) except that elastic constants are taken as $C_{11}(T)=1.0$, $C_{13}(T)=0.2$, $C_{33}(T)=0.5$, $C_{44}(T)=0.6$, $C_{66}(T)=0.8$, $R_1(T)=-0.2$, $C_{11}(T_q)=0.9$, $C_{13}(T_q)=0.3$, $C_{33}(T_q)=0.4$, $C_{44}(T_q)=0.5$, $C_{66}(T_q)=0.6$, $R_1(T_q)=-0.15$, $K_1(T_q)=1.5$, and $K_4(T_q)=0.3$. (c) The same as (a) except that phasons are assumed thermalized. Phason elastic constants are taken as $K_1(T)=0.7$, and $K_4(T)=0.5$.

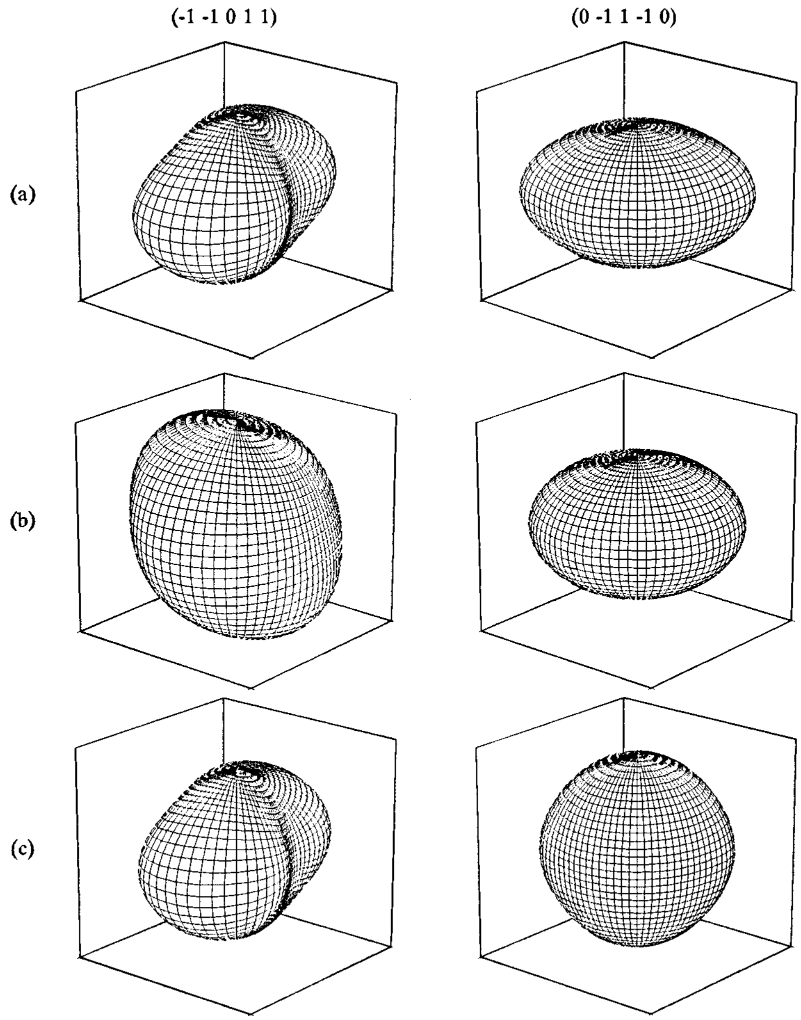

FIG. 3. Comparisons of stereoscopic contours around Bragg spots $(-1\ -1\ 0\ 1\ 1)$ and $(0\ -1\ 1\ -1\ 0)$ with quenched phasons when $T=\frac{1}{3}T_q$ for the case of Laue class 14. Phonon-phason coupling elastic constants are taken as $R_1(T)=0.1$ and $R_1(T_q)=0.15$. The other parameters are taken as follows: (a) $C_{11}(T)=1.0$, $C_{13}(T)=-0.3$, $C_{33}(T)=0.3$, $C_{44}(T)=0.5$, $C_{66}(T)=0.2$, $C_{11}(T_q)=0.9$, $C_{13}(T_q)=-0.2$, $C_{33}(T_q)=0.3$, $C_{44}(T_q)=0.4$, $C_{66}(T_q)=0.3$, $K_1(T_q)=0.6$, and $K_4(T_q)=1.2$; (b) $C_{11}(T)=1.0$, $C_{13}(T)=-0.1$, $C_{33}(T)=0.9$, $C_{44}(T)=0.8$, $C_{66}(T)=0.7$, $C_{11}(T_q)=0.9$, $C_{13}(T_q)=-0.1$, $C_{33}(T_q)=0.7$, $C_{44}(T_q)=0.6$, $C_{66}(T_q)=0.5$ and the same phason elastic constants as those in (a); (c) the same phonon elastic constants as those in (a) and $K_1(T_q)=1.2$, $K_4(T_q)=0.9$.

measured in the plane perpendicular to the periodic direction as Figs. 2(a)–2(c) so that such patterns are insufficient to acquire these elastic constants. Figures 2(d) and 2(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 neighboring equivalent direction with the same conditions as for Fig. 2(a) and they may be used to give information about the other elastic constants that Figs. 2(a)–2(c) cannot present.

The symmetries of diffuse scattering patterns shown in Fig. 2 are consistent with point group 10/mmm. There are two kinds of mirrors in Figs. 2(a)–2(c) besides a tenfold rotation axis along the periodic direction. One is perpendicular to A2P and the other perpendicular to A2D.

As shown in 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 comparisons of stereoscopic contours of constant diffuse scattering intensity around Bragg spots $(-1\ -1\ 0\ 1\ 1)$ and $(0\ -1\ 1\ -1\ 0)$ for quenched phasons when $T=\frac{1}{3}T_q$. In calculation, we consider three sets of elastic constants. Only phonon elastic constants in Fig. 3(b) and phason elastic constants in Fig. 3(c) are changed with respect to those in Fig. 3(a). It is evident that the shape of isointensity contour around reflection $(0\ -1\ 1\ -1\ 0)$ which has large $\mathbf{Q}^{\perp}$ component varies greatly in Fig. 3(c) but slightly in Fig. 3(b) in comparison with that in Fig. 3(a) while the very reverse results can be found for reflection $(-1\ -1\ 0\ 1\ 1)$ which has large $\mathbf{Q}^{\parallel}$ component. The fact that peak shapes of Bragg spots with large $\mathbf{Q}^{\perp}$ 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.

Diffuse scattering from Al-Cu-Co decagonal quasicrystals was observed in transmission x-ray Laue pattern[31] and synchrotron x-ray diffraction experiment.[32,33] In these experiments, structural defects, i.e., short-range atomic correlation, give rise to the diffuse scattering, which cannot be accounted for by the theory of thermal diffuse scattering from decagonal quasicrystals presented here.

V. CONCLUSIONS

Explicit formulas for diffuse scattering from decagonal quasicrystals have been derived in terms of the elastic constants. Contours of constant diffuse scattering intensity were calculated to examine the effect of phonon and phason disorders on diffuse scattering from decagonal quasicrystals. The symmetries of diffuse scattering patterns are consistent with corresponding point groups. Unlike ordinary crystals, the anisotropic peak shapes of decagonal quasicrystals vary greatly even for Bragg spots aligned with a given direction in reciprocal space due to the additional phason degrees of freedom. Analysis of peak shapes can be used to acquire numerical values of elastic constants if diffuse scattering patterns can be measured precisely.

ACKNOWLEDGMENT

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

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