Linear elasticity theory of cubic quasicrystals

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With group-representation theory all quadratic invariants and the expressions of elastic energy have been derived for quasicrystals with cubic point-group symmetry. Using the generalized elasticity theory of quasicrystals, we have also obtained the expressions of the generalized Hooke's law and equilibrium for cubic quasicrystals.

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 discovered. The structure of all these quasicrystals have noncrystallographic point-group symmetries, and can be described by the projection method from higher-dimensional periodic lattice. However, a quasiperiodic structure is not necessary to be associated with noncrystallographic point-group symmetry.[5] Indeed, a quasiperiodic structure with cubic group symmetry has been discovered in the rapid solidified $V_6Ni_{16}Si_7$ alloy.[6–8]

As is well known, in the density wave picture describing quasiperiodic structure, a convenient parametrization of the phase is given by[9]

$$\Phi_n = \mathbf{G}_n^{\parallel}\cdot\mathbf{u} + \alpha G_n^{\perp}\cdot\mathbf{w} , \tag{1.1}$$

where the vector $\mathbf{G}_n^{\parallel}$ and the phonon displacement $\mathbf{u}$ are in the physical space V_E and the reciprocal vector $\mathbf{G}_n^{\perp}$ and the phason displacement $\mathbf{w}$ are in the perpendicular space V_I. For the quasicrystals with noncrystallographic point-group symmetry, as mentioned above, V_E and V_I transform under different irreducible representations. But, according to Janssen's theory on the classification of symmetry operations for n-dimensional periodic and quasiperiodic structure,[10] for the cubic quasicrystals which have crystallographic point-group symmetry, both V_E and V_I can be transformed under the same irreducible representation, which will induce some elastic behavior different from quasicrystals with noncrystallographic point-group symmetry.

The number of independent elastic constants and the expressions for elastic energy as the function of gradients in $\mathbf{u}$ and $\mathbf{w}$ have been derived for pentagonal and icosahedral[9] phases and octagonal and dodecagonal phases.[11] In this paper, we will give the expressions of all quadratic invariants and the elastic energy to quadratic order for the cubic quasicrystals using group-representation theory, and derive the expressions of the Hooke's law and equilibrium equation according to the generalized elasticity theory for quasicrystals.[12]

II. THE ELASTIC ENERGY OF CUBIC QUASICRYSTALS

The cubic point-group O(432) is a 24-element group with five conjugacy classes and five irreducible representations, two of which (Γ_1,Γ_1') are one-dimensional (1D) and one (Γ_2) two-dimensional (2D) and two (Γ_3,Γ_3') three-dimensional (3D) irreducible representations. The cubic point-group with inversions O_h has 48 elements, 10 conjugacy classes, and 10 irreducible representations. Since O_h is isomorphic to $O\otimes C_2$, i.e., $O_h \cong O\otimes C_2$, all irreducible representations can be obtained from the five representations of O, combined with either $+1$ or -1 for the inversion. Here C_2 is a two-element group (unity and inversion). Three rationally independent reciprocal basis vectors $\mathbf{a}_i^* = a(\delta_{i1},\delta_{i2},\delta_{i3})$, $i=1,2,3$ are along three mutually perpendicular axes. Three other reciprocal basis vectors $\mathbf{a}_i^* = \mu a(\delta_{i4},\delta_{i5},\delta_{i6})$, $i=4,5,6$ have the same directions as $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, and $\mathbf{a}_3^*$, but different lengths from $\mathbf{a}_1^*$, $\mathbf{a}_2^*$, and $\mathbf{a}_3^*$ with an irrational ratio μ. The set of all reciprocal vectors

$$\mathbf{k} = \sum_{i=1}^{6} h_i \mathbf{a}_i^* \tag{2.1}$$

is invariant under the symmetry operators of the cubic point-group O. The action of the generators on the basis vectors is given by

$$\Gamma(\alpha) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix} ,$$
$$\Gamma(\beta) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{2.2}$$

where α is a fourfold rotation along [1 0 0] and β is a threefold rotation along [1 1 1]. This matrix representation Γ is reducible. It can be expressed as the direct sum of two of the irreducible representations Γ_3,

$$\Gamma = \Gamma_3 + \Gamma_3 . \tag{2.3}$$

This means that $\mathbf{G}_n^{\parallel}$ and $\mathbf{u}$ transform under Γ_3 (vector representation), whereas $\mathbf{G}_n^\perp$ and $\mathbf{w}$ transfer also under Γ_3 unlike quasicrystals with noncrystallographic point-group symmetry.[11,12] Consequently, the displacement gradients $\partial_j u_i$ $(i,j=1,2,3)$ and $\partial_j w_i$ $(i,j=1,2,3)$ transform according to their respective direct product representations. With the help of group-representation theory, we can construct all quadratic invariants involving $\partial_j u_i$ and $\partial_j w_i$, and hence find the expression for the elastic energy.

For the phonon field, the nine components of $\partial_j u_i$ transform under

$$\Gamma_3 \otimes \Gamma_3 = \Gamma_1 + \Gamma_2 + \Gamma_3' + \Gamma_3 \ . \tag{2.4}$$

It can be proved that among them three antisymmetric components $\Omega_{12} = \partial_2 u_1 - \partial_1 u_2$, $\Omega_{23} = \partial_3 u_2 - \partial_2 u_3$, and $\Omega_{31} = \partial_1 u_3 - \partial_3 u_1$ span the representation space of Γ_3 corresponding to rigid rotations, which do not contribute to the elastic energy. Therefore, for the phonon field of the cubic quasicrystals, $\partial_j u_i$ can be decomposed into symmetric (S) and antisymmetric (A) parts:

$$\partial_j u_i = E_{ij} + \Omega_{ij} \tag{2.5}$$

with $E_{ij} = (\partial_j u_i + \partial_i u_j)/2$ and $\Omega_{ij} = (\partial_j u_i - \partial_i u_j)/2$. With the group-representation theory, the direct product representation (2.4) can also be expressed as

$$\Gamma_3 \otimes \Gamma_3 = (\Gamma_3 \otimes \Gamma_3)^S + (\Gamma_3 \otimes \Gamma_3)^A \tag{2.6}$$

with $(\Gamma_3 \otimes \Gamma_3)^A = \Gamma_3$. The symmetric components $\partial_1 u_1 + \partial_2 u_2 + \partial_3 u_3$ spans the 1D irreducible representation Γ_1. Since Γ_1 (the identity representation) appears once and only once in the product $\Gamma_1 \otimes \Gamma_1$, it is easily verified that

$$(E_{11} + E_{22} + E_{33})^2 \tag{2.7}$$

is an invariant. Similarly, the pair

$$[(\partial_1 u_1 + \partial_2 u_2 - 2\partial_3 u_3)/\sqrt{6},\ (\partial_1 u_1 - \partial_2 u_2)/\sqrt{2}]$$

spans the 2D irreducible representation Γ_2,

$$(E_{11} + E_{22} - 2E_{33})^2 + 3(E_{11} - E_{22})^2 \tag{2.8}$$

is an invariant. The 3D vector $(\partial_1 u_2 + \partial_2 u_1,\ \partial_1 u_3 + \partial_3 u_1,\ \partial_2 u_3 + \partial_3 u_2)/\sqrt{2}$ spans the 3D irreducible representation Γ_3', which gives the third invariant

$$E_{12}^2 + E_{23}^2 + E_{31}^2 \ . \tag{2.9}$$

In quadratic approximation, the part of the elastic energy density due to the phonon field is a linear combination of these invariants, leading to the form

$$f^u = C_{12}(E_{ii})^2/2 + C_{44} E_{ij} E_{ij} + (C_{11} - C_{12} - 2C_{44})(E_{11}^2 + E_{22}^2 + E_{33}^2)/2 \ . \tag{2.10}$$

As mentioned above, both $\partial_j u_i$ and $\partial_j w_i$ transform under the direct product representation $\Gamma_3 \otimes \Gamma_3$, so that the same elastic behavior can be presumed both for phonon and phason field $\mathbf{u}$ and $\mathbf{w}$. Therefore, the expressions of the invariants and the elastic energy corresponding to the phason field can easily be obtained if we substitute

$$F_{ij} = (\partial_j w_i + \partial_i w_j)/2$$

for E_{ij} in Eqs. (2.7)–(2.10). For example, the expression of the elastic energy contributed by F_{ij} is

$$f^w = K_{12}(F_{ii})^2/2 + K_{44} F_{ij} F_{ij} + (K_{11} - K_{12} - 2K_{44})(F_{11}^2 + F_{22}^2 + F_{33}^2)/2 \ . \tag{2.11}$$

It must be noticed, for the icosahedral, pentagonal, octagonal, decagonal, and dodecagonal quasicrystals with noncrystallographic point-group symmetry, ∂_j and w_j transform under different irreducible representations, and hence $\partial_j w_i$ cannot be decomposed into symmetric and antisymmetric parts. In this case the similarity between Eqs. (2.10) and (2.11) does not exist.

Finally, there are three invariants corresponding to the coupling between E_{ij} and F_{ij}, because they transform under the same irreducible representations:

$$\begin{aligned} &(E_{11} + E_{22} + E_{33})(F_{11} + F_{22} + F_{33}) \ , \\ &(E_{11} + E_{22} - 2E_{33})(F_{11} + F_{22} - 2F_{33}) + 3(E_{11} - E_{22})(F_{11} - F_{22}) \ , \\ &E_{12}F_{12} + E_{23}F_{23} + E_{31}F_{31} \ . \end{aligned} \tag{2.12}$$

Thus, the mixing term in total elastic energy density takes the form

$$f^{uw} = R_1(E_{11}F_{11} + E_{22}F_{22} + E_{33}F_{33}) + R_2(E_{11}F_{22} + E_{11}F_{33} + E_{22}F_{11} + E_{22}F_{33} + E_{33}F_{11} + E_{33}F_{22}) + 4R_3(E_{12}F_{12} + E_{23}F_{23} + E_{31}F_{31}) \ . \tag{2.13}$$

Therefore, the total elastic energy density f is the sum of f^u, f^w, and f^{uw}

$$f = f^u + f^w + f^{uw} \ , \tag{2.14}$$

where f^u, f^w, and f^{uw} are given by Eqs. (2.10), (2.11), and (2.13), respectively. From these equations, it follows that there are nine independent elastic constants in the cubic quasicrystal structure: three coupling $\mathbf{u}$ to $\mathbf{u}$, three coupling $\mathbf{w}$ to $\mathbf{w}$, and three coupling $\mathbf{u}$ to $\mathbf{w}$.

With the matrix representation of the elastic constants,[12] Eq. (2.14) can be written as

$$
\begin{aligned}
f=&\tfrac{1}{2}C_{12}(E_{ii})^2+C_{44}E_{ij}E_{ij}+\tfrac{1}{2}(C_{11}-C_{12}-2C_{44})(E_{11}^2+E_{22}^2+E_{33}^2)+\tfrac{1}{2}K_{12}(F_{ii})^2+K_{44}F_{ij}F_{ij}\\
&+\tfrac{1}{2}(K_{11}-K_{12}-2K_{44})(F_{11}^2+F_{22}^2+F_{33}^2)+R_2(E_{ii})(F_{jj})+2R_3(E_{ij}F_{ij})\\
&+(R_1-R_2-2R_3)(E_{11}F_{11}+E_{22}F_{22}+E_{33}F_{33})\\
=&\frac{1}{2}(E\quad F)\begin{bmatrix} C & R\\ R^T & K\end{bmatrix}\begin{bmatrix} E\\ F\end{bmatrix}\\
=&\tfrac{1}{2}(E_{11},E_{22},E_{33},2E_{23},2E_{31},2E_{12},F_{11},F_{22},F_{33},2F_{23},2F_{31},2F_{12})
\end{aligned}
$$

$$
\times\begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 & R_1 & R_2 & R_2 & 0 & 0 & 0\\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 & R_2 & R_1 & R_2 & 0 & 0 & 0\\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 & R_2 & R_2 & R_1 & 0 & 0 & 0\\
0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & 0 & R_3 & 0 & 0\\
0 & 0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & 0 & R_3 & 0\\
0 & 0 & 0 & 0 & 0 & C_{44} & 0 & 0 & 0 & 0 & 0 & R_3\\
R_1 & R_2 & R_2 & 0 & 0 & 0 & K_{11} & K_{12} & K_{12} & 0 & 0 & 0\\
R_2 & R_1 & R_2 & 0 & 0 & 0 & K_{12} & K_{11} & K_{12} & 0 & 0 & 0\\
R_2 & R_2 & R_1 & 0 & 0 & 0 & K_{12} & K_{12} & K_{11} & 0 & 0 & 0\\
0 & 0 & 0 & R_3 & 0 & 0 & 0 & 0 & 0 & K_{44} & 0 & 0\\
0 & 0 & 0 & 0 & R_3 & 0 & 0 & 0 & 0 & 0 & K_{44} & 0\\
0 & 0 & 0 & 0 & 0 & R_3 & 0 & 0 & 0 & 0 & 0 & K_{44}
\end{bmatrix}
\begin{bmatrix} E_{11}\\ E_{22}\\ E_{33}\\ 2E_{23}\\ 2E_{31}\\ 2E_{12}\\ F_{11}\\ F_{22}\\ F_{33}\\ 2F_{23}\\ 2F_{31}\\ 2F_{12}\end{bmatrix}
\tag{2.15}
$$

III. GENERALIZED HOOKE'S LAW AND EQUILIBRIUM EQUATION

According to the generalized elasticity theory for quasicrystals,[12] the generalized Hooke's law and the static equilibrium equation takes the following forms, respectively:

$$
\begin{bmatrix} T\\ H\end{bmatrix}=\begin{bmatrix} C & R\\ R^T & K\end{bmatrix}\begin{bmatrix} E\\ F\end{bmatrix}
\tag{3.1}
$$

and

$$
\begin{aligned}
&\partial_j T_{ij}+f_i=0\ ,\\
&\partial_j H_{ij}+g_i=0\ ,
\end{aligned}
\tag{3.2}
$$

where **T** and **H** are stress tensors and **f** and **g** are body force densities for the phonon (**T** and **f**) and phason (**H** and **g**) displacements, respectively. The component $\mathbf{T}_{ij}$ possesses the conventional meaning and the component $\mathbf{H}_{ij}$ designates a stress acting on the surface with the outward normal parallel to the X_j axis in V_E and along the X_i axis in V_I. The component g_i is the body force density also along the X_i axis in V_I. Both of them are all necessary in the elasticity theory of quasicrystals to describe the forces needed for overcoming the barriers when the atoms rearrange.

Substituting the matrix in Eq. (2.15) into Eq. (3.1), we can obtain the generalized Hooke's law as follows:

$$
\begin{aligned}
T_{11}=&C_{11}E_{11}+C_{12}E_{22}+C_{12}E_{33}+R_1F_{11}\\
&+R_2F_{22}+R_2F_{33}\ ,\\
T_{22}=&C_{12}E_{11}+C_{11}E_{22}+C_{12}E_{33}+R_2F_{11}\\
&+R_1F_{22}+R_2F_{33}\ ,\\
T_{33}=&C_{12}E_{11}+C_{12}E_{22}+C_{11}E_{33}+R_2F_{11}\\
&+R_2F_{22}+R_1F_{33}\ ,\\
T_{23}=&2C_{44}E_{23}+2R_3F_{23}=T_{32}\ ,\\
T_{31}=&2C_{44}E_{31}+2R_3F_{31}=T_{13}\ ,\\
T_{12}=&2C_{44}E_{12}+2R_3F_{12}=T_{21}\ ,
\end{aligned}
\tag{3.3a}
$$

$$
\begin{aligned}
H_{11}=&R_1E_{11}+R_2E_{22}+R_2E_{33}+K_{11}F_{11}\\
&+K_{12}F_{22}+K_{12}F_{33}\ ,\\
H_{22}=&R_2E_{11}+R_1E_{22}+R_2E_{33}+K_{12}F_{11}\\
&+K_{11}F_{22}+K_{12}F_{33}\ ,\\
H_{33}=&R_2E_{11}+R_2E_{22}+R_1E_{33}+K_{12}F_{11}\\
&+K_{12}F_{22}+K_{11}F_{33}\ ,\\
H_{23}=&2R_3E_{23}+2K_{44}F_{23}=H_{32}\ ,\\
H_{31}=&2R_3E_{31}+2K_{44}F_{31}=H_{13}\ ,\\
H_{12}=&2R_3E_{12}+2K_{44}F_{12}=H_{21}\ .
\end{aligned}
\tag{3.3b}
$$

From Eqs. (3.3) we see that V_E and V_I which are treated as continuum, obey the same constitutive equation, i.e., both of them have the same elastic behavior. This should be expected since they transform under the same irreducible representations.

Substituting Eqs. (3.3a) and (3.3b) into Eq. (3.2), the inhomogeneous partial differential equations satisfied by $\mathbf{u}$ and $\mathbf{w}$ in the cubic quasicrystals can be obtained:

$$
\begin{aligned}
&C_{44}\nabla^2 u_1+(C_{11}-C_{12}-2C_{44})\partial_1\partial_1 u_1+(C_{12}+C_{44})\frac{\partial}{\partial x}(\nabla\cdot\mathbf{u})\\
&\qquad +R_3\nabla^2 w_1+(R_1-R_2-2R_3)\partial_1\partial_1 w_1+(R_2+R_3)\frac{\partial}{\partial x}(\nabla\cdot\mathbf{w})+f_1=0\ ,\\
&C_{44}\nabla^2 u_2+(C_{11}-C_{12}-2C_{44})\partial_2\partial_2 u_2+(C_{12}+C_{44})\frac{\partial}{\partial y}(\nabla\cdot\mathbf{u})\\
&\qquad +R_3\nabla^2 w_2+(R_1-R_2-2R_3)\partial_2\partial_2 w_2+(R_2+R_3)\frac{\partial}{\partial y}(\nabla\cdot\mathbf{w})+f_2=0\ ,\\
&C_{44}\nabla^2 u_3+(C_{11}-C_{12}-2C_{44})\partial_3\partial_3 u_3+(C_{12}+C_{44})\frac{\partial}{\partial z}(\nabla\cdot\mathbf{u})\\
&\qquad +R_3\nabla^2 w_3+(R_1-R_2-2R_3)\partial_3\partial_3 w_3+(R_2+R_3)\frac{\partial}{\partial z}(\nabla\cdot\mathbf{w})+f_3=0\ ,\\
&R_3\nabla^2 u_1+(R_1-R_2-2R_3)\partial_1\partial_2 u_1+(R_2+R_3)\frac{\partial}{\partial x}(\nabla\cdot\mathbf{u})\\
&\qquad +K_{44}\nabla^2 w_1+(K_{11}-K_{12}-2K_{44})\partial_1\partial_1 w_1+(K_{12}+K_{44})\frac{\partial}{\partial x}(\nabla\cdot\mathbf{w})+g_1=0\ ,\\
&R_3\nabla^2 u_2+(R_1-R_2-2R_3)\partial_2\partial_2 u_2+(R_2+R_3)\frac{\partial}{\partial y}(\nabla\cdot\mathbf{u})\\
&\qquad +K_{44}\nabla^2 w_2+(K_{11}-K_{12}-2K_{44})\partial_2\partial_2 w_2+(K_{12}+K_{44})\frac{\partial}{\partial y}(\nabla\cdot\mathbf{w})+g_2=0\ ,\\
&R_3\nabla^2 u_3+(R_1-R_2-2R_3)\partial_3\partial_3 u_3+(R_2+R_3)\frac{\partial}{\partial x}(\nabla\cdot\mathbf{u})\\
&\qquad +K_{44}\nabla^2 w_3+(K_{11}-K_{12}-2K_{44})\partial_3\partial_3 w_3+(K_{12}+K_{44})\frac{\partial}{\partial z}(\nabla\cdot\mathbf{w})+g_3=0\ ,
\end{aligned}
\tag{3.4}
$$

IV. CONCLUSION

The main results obtained are as follows.

(1) There are nine independent elastic constants: three belong to the phonon field, three to the phason field, and three to the coupling between $\mathbf{u}$ and $\mathbf{w}$.

(2) As distinguished from quasicrystals with noncrystallographic point-group symmetries, the elastic behavior of the phason field in the cubic quasicrystals has analogy to that of the phonon field: (i) their matrices of the elastic constant, expressions of Hooke's law and equilibrium equations, are of the same form, (ii) the gradient tensor $\partial_j w_i$ can also be decomposed into symmetric and antisymmetric parts, and the latter can also be neglected like $\partial_j u_i$, and (iii) $H_{ij}=H_{ji}$, like $T_{ij}=T_{ji}$. It should be expected that these results are also applicable for other quasicrystals with the n-dimensional point group, the representation space of which can be reduced to the direct sum of two equivalent irreducible subspaces.

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