

Nonlinear elastic properties of decagonal quasicrystals

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Quasicrystals have both positional and orientational long-range order. Thus, they are essentially anisotropic. However, both theory and experiment show that ordinary linear elastic property (linear phonon elasticity) is isotropic for quasicrystals. To detect the quasicrystal anisotropy the nonlinear elasticity should be discussed. In this paper the nonlinear elastic properties are analyzed for decagonal quasicrystals. All the third-order elastic constants (including phason strain) are determined for all symmetries of decagonal quasicrystals. The nonlinear elastic properties due to the coupling between phonons and phasons may reveal the anisotropic structure of decagonal quasicrystals by Hermann's theorem.

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I. INTRODUCTION

Since the discovery of quasicrystals (QCs), their linear elastic properties were extensively investigated.¹ It shows that within linear phonon elasticity QCs behave essentially like isotropic media. The experimental measurements have also confirmed this point.²⁻⁶ As is well known, QCs are new types of solids, which possess positional and orientational long-range order (quasiperiodicity) and may have a crystallographically forbidden point-group symmetry. Accordingly one could expect the physical behavior of a quasicrystal not to be isotropic as in a glass but in principle to be anisotropic as in a crystal. However, the commonly observed properties are isotropic due to their low tensorial rank and do not reveal the anisotropic structure of QCs.^{7,8} To detect the QC anisotropy some people have studied nonlinear elastic properties and phonon-phason coupling of the icosahedral QC.⁹⁻¹¹ Meanwhile, all third-order elastic constants have already been determined for the icosahedral QCs.¹² Besides, the pure phonon third-order elastic constants have also been calculated for decagonal QCs.¹³ In this paper we would like to determine all third-order elastic constants (including phason strain) of decagonal QCs. Decagonal QCs are two-dimensional (2D) QCs, which have a periodicity along one axis (tenfold axis) but quasiperiodicity in the 2D plane perpendicular to it. There are two Laue classes and seven point groups—10, $\bar{1}0$, $10/m$, $10mm$, 1022 , $\bar{1}0m2$, $10/mmm$ in the decagonal QC.¹ The first three groups belong to Laue 13, the other to Laue 14 (the number of Laue classes is the same as in Ref. 1). The results show that there are 40 independent third-order elastic constants (10 due to phonon field, 6 due to phason field, 10 due to phonon-phonon-phason coupling, and 14 due to phonon-phason-phason coupling) for Laue 13 and 27 independent third-order elastic constants (9 due to phonon field, 3 due to phason field, 5 due to phonon-phonon-phason coupling and 10 due to phonon-phason-phason coupling) for Laue 14, respectively. According to Hermann's theorem,^{7,8} the nonlinear elasticity due to the coupling between phonons and phasons may observe anisotropic structure of decagonal QCs. The following section is devoted to deducing those invariants. All independent third-order elastic constants are tabulated and are given in Table III. Conclusions are given in Sec. III.

II. GENERALIZED ELASTIC THEORY OF DECAGONAL QCS

In the higher-dimensional description of QCs, a dD QC with Fourier modulus of rank n can be generated by intersection an nD space V ($V=V_E+V_I$) by 3D physical subspace V_E . Consequently, an nD displacement vector $\tilde{\mathbf{u}}$ in V , when projected upon V_E and V_I , becomes a direct sum:

$$\tilde{\mathbf{u}} = \mathbf{u}^{\parallel} + \mathbf{u}^{\perp} = \mathbf{u} + \mathbf{w} \quad (1)$$

where \mathbf{u} (phonon displacement) is a 3D vector in V_E in which a vector transforms under the vector representation (Γ_A) of the symmetry group of the structure considered and \mathbf{w} is an $(n-3)D$ vector (phason displacement) in V_I (perpendicular space) in which a vector transforms under another irreducible representation (Γ_B). For a decagonal QC n equals 5. The corresponding phonon strain \mathbf{E} has its components of the symmetric form $E_{ij} = \frac{1}{2}(\partial_j u_i + \partial_i u_j)$ and the corresponding phason strain \mathbf{W} has its components of form $W_{\alpha i} = \partial_i w_{\alpha}$, where Latin letters i, j, k, \dots , are used for indices of 3D phonon displacement vectors, taking on the values 1, 2, 3 and Greek letters $\alpha, \beta, \gamma, \dots$, for indices of 2D phason displacement vectors, taking on the values 1, 2.

Then the elastic energy density F which is a function of phonon and phason strains can be expanded into the Taylor series in the vicinity of $E_{ij}=0$ and $W_{\alpha i}=0$ to third order:

$$\begin{aligned} F(E_{pq}, W_{\mu\nu}) = & \frac{1}{2} C_{ijkl} E_{ij} E_{kl} + \frac{1}{2} K_{\alpha i \beta j} W_{\alpha i} W_{\beta j} + R_{ij\alpha k} E_{ij} W_{\alpha k} \\ & + \frac{1}{6} C_{ijklmn} E_{ij} E_{kl} E_{mn} + \frac{1}{6} K_{\alpha i \beta j \gamma k} W_{\alpha i} W_{\beta j} W_{\gamma k} \\ & + \frac{1}{2} R_{ijkl\alpha m}^{(1)} E_{ij} E_{kl} W_{\alpha m} + \frac{1}{2} R_{ij\alpha k \beta l}^{(2)} E_{ij} W_{\alpha k} W_{\beta l}, \end{aligned} \quad (2)$$

where

$$C_{ijkl} = \left(\frac{\partial^2 F}{\partial E_{ij} \partial E_{kl}} \right)_0, \quad K_{\alpha i \beta j} = \left(\frac{\partial^2 F}{\partial W_{\alpha i} \partial W_{\beta j}} \right)_0$$

and

TABLE I. Laue classes, point groups, dimension of symmetrized space, and the numbers of invariants of third-order elastic constants for decagonal QCs.

Laue classes	Point groups	Third-order elastic tensors	Dimension of symmetrized space	Numbers of independent invariants
13	10, $\overline{10}$, 10/ <i>m</i>	C_{ijklmn}	56	10
		$K_{\alpha i \beta j \gamma k}$	56	6
		$R_{ijklam}^{(1)}$	126	10
		$R_{ijak\beta l}^{(2)}$	126	14
14	$10mm$, 1022 , $\overline{10}m2$, $10/mmm$	C_{ijklmn}	56	9
		$K_{\alpha i \beta j \gamma k}$	56	3
		$R_{ijklam}^{(1)}$	126	5
		$R_{ijak\beta l}^{(2)}$	126	10

$$R_{ijak} = \left(\frac{\partial^2 F}{\partial E_{ij} \partial W_{ak}} \right)_0 \quad (3)$$

are second-order elastic constants of phonon field, phason field and phonon-phason coupling, respectively. Similarly,

$$C_{ijklmn} = \left(\frac{\partial^3 F}{\partial E_{ij} \partial E_{kl} \partial E_{mn}} \right)_0$$

and

$$K_{\alpha i \beta j \gamma k} = \left(\frac{\partial^3 F}{\partial W_{\alpha i} \partial W_{\beta j} \partial W_{\gamma k}} \right)_0 \quad (4)$$

are the third-order elastic constants of phonon and phason fields, respectively, and

$$R_{ijklam}^{(1)} = \left(\frac{\partial^3 F}{\partial E_{ij} \partial E_{kl} \partial W_{am}} \right)_0$$

and

$$R_{ijak\beta l}^{(2)} = \left(\frac{\partial^3 F}{\partial E_{ij} \partial W_{ak} \partial W_{\beta l}} \right)_0 \quad (5)$$

are the third-order elastic constants associated with phonon-phonon-phason coupling and phonon-phason-phason coupling, respectively.

By using group representation theory all invariants of these elastic constants can be determined. As we know, the number of independent tensor components is equal to the number of times that the identity representation is contained in this tensor representation, e.g.,

$$n = \frac{1}{|G|} \sum_{g \in F} \bar{\chi}(g) \quad (6)$$

where $|G|$ is the order of G , $\bar{\chi}$ is the character of the tensor representation. Once the characters of C_{ijklmn} , $K_{\alpha i \beta j \gamma k}$, $R_{ijklam}^{(1)}$, and $R_{ijak\beta l}^{(2)}$ are calculated for any $g \in G$, the number of independent components of all nonlinear elastic tensors are immediately obtained from Eq. (6). The formulas for calculating the characters of C_{ijklmn} , $K_{\alpha i \beta j \gamma k}$, $R_{ijklam}^{(1)}$, and $R_{ijak\beta l}^{(2)}$ have already been given in our earlier work.¹⁴ Unfortunately in Ref. 14 a mistake was made in calculating the dimension of symmetric space and the number of independent tensor components for $K_{\alpha i \beta j \gamma k}$, $R_{ijklam}^{(1)}$, and $R_{ijak\beta l}^{(2)}$ where the phason strain $W_{\alpha i}$ was considered to be independent of z -components. The right results are given in Table I.

The determination of explicit forms for these invariants is much more complicated than counting their number. As an example, we consider $K_{\alpha i \beta j \gamma k}$ for decagonal QCs with the $10mm$ symmetry. This point group has eight irreducible representations (cf. Table II), four of which are one-dimensional

TABLE II. Characters of $10mm$ symmetry.

$10mm$	e	2α	$2\alpha^2$	$2\alpha^3$	$2\alpha^4$	α^5	5β	$5\alpha\beta$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	-1	-1
Γ_3	1	-1	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	1	1	-1	1
Γ_5	2	τ	$\tau-1$	$1-\tau$	$-\tau$	-2	0	0
Γ_6	2	$\tau-1$	$-\tau$	$-\tau$	$\tau-1$	2	0	0
Γ_7	2	$1-\tau$	$-\tau$	τ	$\tau-1$	-2	0	0
Γ_8	2	$-\tau$	$\tau-1$	$\tau-1$	$-\tau$	2	0	0

TABLE III. Independent third-order elastic constants for decagonal QCs.

Laue classes	Point group	Third-order elastic constants	Independent invariants
13	10, $\overline{10}$ 10/m	C_{ijklmn}	$C_{111}=C_{222}$ $C_{112}=C_{122}$ $C_{113}=C_{223}$ C_{333} C_{123} $C_{144}=C_{255}$ $C_{155}=C_{244}$ $C_{334}=C_{355}$ $C_{133}=C_{233}$ $C_{145}=-C_{245}=C_{446}=-C_{556}$ $C_{166}=C_{266}=\frac{1}{4}(C_{111}-C_{222})$ $C_{366}=\frac{1}{2}(C_{113}-C_{123})$ $C_{456}=\frac{1}{2}(C_{155}-C_{144})$
		$K_{ai\beta j\gamma k}$	$K_{111}=K_{116}$ $K_{135}=-K_{235}=K_{556}=-K_{336}=K_{455}=-K_{334}$ $K_{222}=K_{244}$ $K_{356}=K_{345}=-K_{155}=K_{255}=K_{133}=-K_{233}$ $K_{116}=K_{444}$ $K_{224}=K_{666}$ $K_{124}=-K_{226}=-K_{446}=\frac{1}{3}K_{444}$ $K_{114}=K_{446}=-K_{126}=-\frac{1}{3}K_{666}$ $K_{122}=K_{144}=-K_{126}=-\frac{1}{3}K_{111}$ $K_{112}=K_{226}=-K_{146}=-\frac{1}{3}K_{222}$
		$R_{ijklam}^{(1)}$	$R_{111}=-R_{222}$ $R_{441}=R_{442}=-R_{454}=-R_{456}=-R_{551}=-R_{552}$ $R_{112}=-R_{221}$ $R_{131}=R_{132}=-R_{231}=-R_{232}=-R_{364}=R_{366}$ $R_{116}=R_{224}$ $R_{143}=-R_{243}$ $R_{155}=-R_{255}=-R_{465}=R_{563}$ $R_{226}=R_{114}$ $R_{444}=-R_{446}=-R_{451}=-R_{452}=-R_{554}=R_{556}$ $R_{134}=-R_{136}=-R_{234}=R_{236}=R_{361}=R_{362}$ $R_{145}=-R_{245}=-R_{153}=R_{253}=R_{463}=R_{565}$ $R_{121}=-R_{122}=R_{661}=-R_{662}=-\frac{1}{2}(R_{111}-R_{112})$ $R_{124}=R_{126}=R_{663}=-R_{666}=-\frac{1}{2}(R_{116}+R_{226})$ $R_{166}=-R_{264}=\frac{1}{4}(3R_{111}-R_{112})$ $R_{226}=-R_{164}=\frac{1}{4}(-R_{111}+3R_{112})$ $R_{161}=R_{262}=-\frac{1}{4}(3R_{116}+R_{226})$ $R_{162}=R_{261}=\frac{1}{4}(R_{116}-3R_{226})$
$R_{ijak\beta l}^{(2)}$	$R_{111}=R_{244}$ $R_{122}=R_{266}$ $R_{222}=R_{166}$ $R_{211}=R_{144}$ $R_{135}=R_{235}$ $R_{312}=-R_{346}$ $R_{335}=R_{311}=R_{334}=R_{366}=R_{322}$ $R_{525}=-R_{534}=-R_{413}=R_{423}=R_{456}$ $R_{556}=-R_{513}=R_{523}=R_{434}=-R_{425}$ $R_{611}=-R_{644}=R_{114}=-R_{214}$ $R_{622}=-R_{666}=-R_{126}=R_{226}$		
14	10mm, $\overline{10}22$, $\overline{10}m2$, 10/mmm	C_{ijklmn}	$C_{111}=C_{222}$ $C_{112}=C_{122}$ $C_{113}=C_{223}$ C_{333} C_{123} $C_{144}=C_{255}$ $C_{155}=C_{244}$ $C_{334}=C_{355}$ $C_{133}=C_{233}$ $C_{166}=C_{266}=\frac{1}{4}(C_{111}-C_{222})$ $C_{366}=\frac{1}{2}(C_{113}-C_{123})$ $C_{456}=\frac{1}{2}(C_{155}-C_{144})$
		$K_{ai\beta j\gamma k}$	$K_{444}=-K_{666}=K_{116}=-K_{224}=-3K_{126}=-3K_{226}$ $=3K_{114}=3K_{124}=3K_{446}=-3K_{466}$ $K_{111}=-K_{222}=K_{166}=-K_{244}=-3K_{146}=3K_{246}$ $=3K_{112}=-3K_{122}=-3K_{144}=3K_{266}$ $K_{135}=-K_{235}=K_{556}=-K_{336}=K_{455}=-K_{334}$
		$R_{ijklam}^{(1)}$	$R_{111}=-R_{222}$ $R_{441}=R_{442}=-R_{454}=-R_{456}=-R_{551}=-R_{552}$ $R_{112}=-R_{221}$ $R_{131}=R_{132}=-R_{231}=-R_{232}=R_{364}=R_{366}$ $R_{143}=-R_{243}$ $R_{155}=-R_{255}=-R_{465}=R_{563}$ $R_{121}=-R_{122}=R_{661}=-R_{662}=-\frac{1}{2}(R_{111}-R_{112})$ $R_{166}=-R_{264}=\frac{1}{4}(3R_{111}-R_{112})$ $R_{226}=-R_{164}=\frac{1}{4}(-R_{111}+3R_{112})$
$R_{ijak\beta l}^{(2)}$	$R_{111}=R_{222}=R_{244}=R_{166}$ $R_{122}=R_{211}=R_{144}=R_{266}$ R_{355}		

rotational symmetry, they are fundamentally anisotropic and at the macroscopic level there should be some anisotropic physical properties. According to Hermann's theorem the minimal tensorial rank which is necessary to reveal the anisotropy of a symmetry is related to the order of the symmetry rotation.^{7,8} However, the symmetry of QCs is always so high that mostly macroscopic properties are isotropic unless they are described by a tensor with rank $N \geq 5$ for icosahedral QCs or $N \geq 10$ for decagonal QCs. In particular, QCs have additional phason degrees of freedom which are frozen at room temperature but excited at high temperature. The phason displacement can be seen as a tensor of high rank since it does not transform under the vector representation Γ_A but the irreducible representation Γ_B . The phason displacement of decagonal or icosahedral QCs is a tensor of rank 3. It is easy to find out that the elastic constants C_{ijklmn} and R_{ijk} are

tensors of rank 6. Thus the third-order nonlinear phonon elastic properties and linear elastic properties at high temperature due to phonon-phason coupling of icosahedral QCs are expected to be anisotropic.^{8,10} Such conclusion has been confirmed experimentally.⁹ Unlike for icosahedral QCs, for decagonal QCs neither of them would be anisotropic due to their low tensorial rank which is verified by Rochal *et al.* who showed the dispersions corresponding to the elastic waves do not depend on the wave vector direction. So the decagonal QC anisotropy may be revealed only by the third-order elastic constants $R_{ijk\beta j}^{(2)}$ which is a tensor of rank 10. Following Rochal *et al.* the angular anisotropy of acoustic phonon velocity and attenuation coefficient of decagonal QCs at high temperature due to phonon-phason coupling in the nonlinear elastic domain may be observed in experiments.

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