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The physical property tensors of one-dimensional quasicrystals*

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According to the group representation theory, we derive the character formulae of representation-matrices of the physical property tensors for the one-dimensional (1D) quasicrystals. Based on this, we have calculated the numbers of independent components of representation-matrices for thermal expansion coefficient tensors, piezoelectric coefficient tensors and elastic constant tensors under 31 point-groups for the 1D quasicrystals. Moreover, we have deduced the particular matrix forms of these tensors under the 31 point-groups. This is an important complement of quasicrystal physical property.

Keywords: quasicrystal, thermal expansion coefficient, piezoelectric coefficient
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1. Introduction

Shechtman *et al*[1] discovered the fivefold symmetry in the diffraction pattern of Al–Mn alloys and first claimed that there is a new structure of solid state in nature, which is like a crystal having long-range translational order and long-range orientational order. However, its translational order is not periodic. Levine and Steinhardt[2,3] studied this kind of new structure order and named it a quasiperiodic crystal, i.e. quasicrystal. Since then, two-dimensional (2D) decagonal quasicrystals and dodecagonal quasicrystals have been successively discovered.[4−6] In 1988, He *et al*[7] first found one-dimensional (1D) quasicrystals derived from the 2D decagonal quasicrystals in rapidly solidified Al–Ni–Si, Al–Cu–Mn, and Al–Cu–Co alloys. Here a 1D quasicrystal is a three-dimensional (3D) physical body with one quasiperiodic direction and one periodic plane. In 1990, Tsai *et al*[8] and Yang *et al*[9] reported the discovery of some stable 1D quasicrystals in the Al–Cu–Fe–Mn systems. Zhang and Kuo[10] described various 1D quasicrystals by adding linear phason strain to the decagonal quasicrystals. Wang and Qin[11] systematically discussed the point and space groups, Laue class, and elastic behaviours for 1D quasicrystals. However, their thermodynamic properties such as the piezoelectric and the thermal-expansion effects have not been studied yet. On the other hand, it is very interesting to investigate the thermal-expansion effect and the piezoelectric effect for a new kind of material.[12,13] In the present paper, we utilize density of wave to describe the phasons[14−19] and study the phasons' effect on the physical property of 1D quasicrystals. According to the Laudou phenomenological theory and group representation theory, we derive the character formulae of the representation matrices and calculate the numbers of independent components of physical-property tensors for 1D quasicrystals. Starting with the generated matrices of point-groups and using the Neumann theorem, we deduce the matrix forms of thermal-expansion coefficient and piezoelectric coefficient tensors under 31 point groups of 1D quasicrystals. Finally, we discuss the difference between the physical property tensors of the quasicrystals and those of the periodic crystals. The present results are a meaningful complement of the quasicrystal physical property tensors and they will provide a theoretical guidance for developing the applications of quasicrystals.

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2. The character formulae of the general representation matrices of 1D quasicrystals

In a periodic structure, let $F_{ij\ldots l}$ represent a component of a tensor of rank n in 3D space; the total number of such components is 3^n. In general, they are independent of each other. If $\hat{A}$ is a coordinate-transformation matrix, the relationship between components $F'_{i'j'k'\ldots l'}$ and $F_{ijk\ldots l}$ is

$$F'_{i'j'k'\ldots l'} = (\hat{A}\times\hat{A}\times\cdots\times\hat{A})_{ijk\ldots l,i'j'k'\ldots l'}F_{ijk\ldots l}, \quad (1)$$

where $F_{ijk\ldots l}$ are related to the old coordinate system and $F'_{i'j'k'\ldots l'}$ to the new system. In addition, the direct product $\hat{\Gamma}(g) = \hat{A}\times\hat{A}\times\cdots\times\hat{A}$ spans a 3^n-dimensional representation space of the symmetry group G. In general, it is reducible. The character of this tensor representation can be calculated by the following formula:

$$\chi(g) = \mathrm{Tr}\hat{\Gamma}(g) = [\mathrm{Tr}\hat{A}(g)]^n. \quad (2)$$

The $\Gamma(g)$ can be reduced to the direct sum of some irreducible representations. The number a_i of the ith irreducible representation $\Gamma^{(i)}(g)$ is determined by

$$a_i = \frac{1}{|G|}\sum_{g\in G}\chi(g)\overline{\mathrm{Tr}\Gamma^{(i)}(g)}, \quad (3)$$

where $|G|$ is the order of group G and the over-bar means the complex conjugation. As we know, the symmetry of a physical property tensor is determined by the macro-symmetry of the material considered, so the number of independent components of the tensor is fixed for a given material. In other words, every independent component will be transformed under identity representation. This means that the number of independent components is just the number a_1 of the identity representation (Γ_1) in the direct representation. Therefore, the basic formula for calculating the number of independent components is

$$a_1 = \frac{1}{|G|}\sum_{g\in G}\chi(g), \quad (4)$$

where $\chi(g)$ is a character of group-element g in a physical-property tensor's representation-matrix. For a 1D quasicrystal, it can be obtained by projecting a four-dimensional (4D) periodic structure onto a 3D physical subspace. Let $\tilde{\boldsymbol{u}}$ be a position vector in the 4D space, $\boldsymbol{u}$ and $\boldsymbol{w}$ its projections in the physical subspace (V_E) and the complementary subspace (V_I), respectively; hence

$$\tilde{\boldsymbol{u}} = \boldsymbol{u} + \boldsymbol{w}, \quad (5)$$

where $\boldsymbol{u}$ transforms under a 3D irreducible representation $\Gamma(A)$, whereas $\boldsymbol{w}$ under a 1D irreducible representation $\Gamma(B)$. Correspondingly, the phonon strains E_{ij} transform under the operator $\hat{A}(g)$ and the phason strains W_{ij} under the $\hat{B}(g)$ operator. We use subscripts $i, j, k, l, m, n, \ldots$ for coordinate components in V_E and subscripts α , β , $\gamma, \ldots$ for coordinate components in V_I, as well as use the notation $\{\ldots\}$ to represent that the subscripts in { } can commute with each other. It is proven that the physical property tensors in quasicrystals may be classified as follows: $F_{ij}, F_{ijk}, F_{ijkl}, \ldots, F_{\alpha i}, F_{i\alpha j}, F_{ik\beta l}, F_{\alpha j\beta l}, \ldots$ Now, let A and B indicate the coordinate transformation matrices of the 3D physical subspace and the 1D complementary subspace, respectively. If the n-fold axis is along the z direction, the transformation matrix of the 3D physical subspace is

$$A(g) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & \pm 1 \end{pmatrix},$$
$$\chi_A(g) = 2\cos\phi \pm 1, \quad (6)$$

and that of 1D complementary subspace is

$$B = \pm 1, \quad \chi_B(g) = \pm 1, \quad (7)$$

where $\phi = 2\pi k/N$ (k=0, 2,..., N–1; N=1, 2, 3, 4, 6) stands for a rotation angle corresponding element g ($g \in G$), '+' represents a real rotation, and '–' a reflective one. According to the group theory, we can obtain the representation matrices ($\Gamma(g)$) and the character formulae of physical-property tensors of 1D quasicrystals in Ref.[20].

3. The numbers of independent components of 1D quasicrystal tensors

The corresponding relationship between the physical property tensors and the general tensors for 1D quasicrystals have been shown in Ref.[20]. According to the conventions in crystallography, the point-groups, which would become identical when a centre of symmetry is added, belong to the same Laue class. It is obvious that all the elastic properties and thermal expansion properties possess intrinsic centrosymmetry, and hence all point groups belonging to the same Laue class have the same elastic and thermal

expansion properties. Thus we can only discuss the numbers of independent elastic constants and thermal expansion coefficients for ten Laue classes of 1D quasicrystals. But, for the piezoelectric effects, because there is no centro-symmetry we must derive the numbers of independent components of the piezoelectric coefficient tensors under all point-groups of 1D quasicrystals. Now, substituting the rotation angle ϕ of each element g of corresponding point groups into the above formulae, we can obtain the characters of the seven types of physical-property tensors' representation matrices. Then, using Eq.(4) we can easily calculate the numbers of independent components a_1. We have computed the numbers of independent components of the physical-property tensors under 31 point-groups as listed in Table 1, where the numbers of independent elastic constants are the same as the results computed by Wang and Qin.[11]

Table 1. Systems, Laue class, point-group, numbers of independent thermal-expansion coefficients (ITEC), piezoelectric coefficients (IPC) and elastic constants (IEC).

System	Laue class	Point group	Numbers of ITEC, IPC, IEC						
			$n_{\alpha(1)}$	$n_{\alpha(2)}$	$n_{d(1)}$	$n_{d(2)}$	n_C	n_K	n_R
Triclinic	$\bar{1}$	1	6	3	18	9	21	6	18
		$\bar{1}$			0	0			
Monoclinic	$2/m_h$	2	4	1	8	5	13	4	8
		m_h			10	5			
		$2/m_h$			0	0			
	$2_h/m$	2_h	4	2	8	4	13	4	10
		m			10	4			
		$2_h/m$			0	0			
Orthorhombic	mmm_h	2_h2_h2	3	1	3	2	9	3	5
		$mm2$			5	3			
		2_hmm_h			0	0			
		mmm_h			0	0			
Tetragonal	$4/m_h$	4	2	1	4	3	7	2	4
		$\bar{4}$			4	2			
		$4/m_h$			0	0			
	$4/m_hmm$	42_h2_h	2	1	1	1	6	2	3
		$4mm$			3	2			
		$\bar{4}2_hm$			2	1			
		$4/m_hmm$			0	0			
Trigonal	$\bar{3}$	3	2	1	6	3	7	2	6
		$\bar{3}$			0	0			
	$\bar{3}m$	32_h	2	1	2	1	6	2	4
		$3m$			4	2			
		$\bar{3}m$			0	0			
Hexagonal	$6/m_h$	6	2	1	4	3	5	2	4
		$\bar{6}$			0	0			
		$6/m_h$			0	0			
	$6/m_hmm$	62_h2_h	1	1	1	1	5	2	3
		$6mm$			3	2			
		$\bar{6}m2_h$			1	0			
		$6/m_hmm$			0	0			

4. The matrix forms of the physical property tensors for the 1D quasicrystals

The physical-property tensors relevant to mechanical quantity are elastic constant, thermal expansion coefficient and piezoelectric coefficient tensors, in which the matrix forms of elastic constant tensors have been discussed in detail.[11] Therefore, we only need to study the matrix forms about thermal-expansion coefficient tensors $(\alpha^{(1)}, \alpha^{(2)})$ and

piezoelectric ones $(d^{(1)}, d^{(2)})$ for 1D quasicrystals. Owing to the thermal expansion property possessing intrinsic centro-symmetry, its tensors are the same for the point groups belonging to the same Laue class, so we only derived the matrix forms of thermal expansion coefficients under the ten Laue classes for 1D quasicrystals. But, for the piezoelectric coefficient tensors, we need to calculate the matrix forms under all the point groups of 1D quasicrystals. After knowing that $\alpha_{ij}^{(1)}$, $d_{ijk}^{(1)}$, $\alpha_{ij}^{(2)}$ and $d_{ijk}^{(2)}$ transform under $A_{ii'}A_{jj'}$, $A_{ii'}A_{jj'}A_{kk'}$, $B_{ii'}A_{jj'}$ and $A_{ii'}B_{jj'}A_{kk'}$, respectively, we can use the generated matrices of each group to replace the matrix A, and ± 1 to replace the matrix B. Then, according to the Neumann theorem, we derive the matrix forms of $\alpha^{(1)}$, $\alpha^{(2)}$, $d^{(1)}$ and $d^{(2)}$ under all point groups of 1D quasicrystals as follows.

4.1. The matrix forms of the thermal expansion coefficient tensors

4.1.1. Triclinic system

In the triclinic 1D quasicrystal system, the point group may be 1 or $\bar{1}$, the matrix of $\alpha^{(1)}$ has six independent components, i.e.

$$\alpha^{(1)} = \begin{pmatrix} \alpha_{11}^{(1)} & \alpha_{12}^{(1)} & \alpha_{13}^{(1)} \\ \alpha_{12}^{(1)} & \alpha_{22}^{(1)} & \alpha_{23}^{(1)} \\ \alpha_{13}^{(1)} & \alpha_{23}^{(1)} & \alpha_{33}^{(1)} \end{pmatrix}, \tag{8}$$

and the matrix of $\alpha^{(2)}$ has three independent components, i.e.

$$\alpha^{(2)} = \begin{pmatrix} 0 & 0 & \alpha_{13}^{(2)} \\ 0 & 0 & \alpha_{23}^{(2)} \\ \alpha_{13}^{(2)} & \alpha_{23}^{(2)} & \alpha_{33}^{(2)} \end{pmatrix}. \tag{9}$$

4.1.2. Monoclinic system

In the monoclinic 1D quasicrystal system, there are two Laue classes, i.e. $2/m_h(2, m_h, 2/m_h)$ and $2_h/m(2_h, m, 2_h/m)$. For the point group of $2, m_h$ and $2/m_h$, the unique axis is the z axis. The matrices of $\alpha^{(1)}$ and $\alpha^{(2)}$ are

$$\alpha^{(1)} = \begin{pmatrix} \alpha_{11}^{(1)} & \alpha_{12}^{(1)} & 0 \\ \alpha_{12}^{(1)} & \alpha_{22}^{(1)} & 0 \\ 0 & 0 & \alpha_{33}^{(1)} \end{pmatrix},$$
$$\alpha^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \alpha_{33}^{(1)} \end{pmatrix}; \tag{10}$$

for 2_h, m and $2_h/m$ point groups, the unique axis lies in the horizontal plane, say along the y axis, the matrix A is

$$A = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad B = -1. \tag{11}$$

Thus, the matrix of α_{ij} is

$$\alpha^{(1)} = \begin{pmatrix} \alpha_{11}^{(1)} & 0 & \alpha_{13}^{(1)} \\ 0 & \alpha_{22}^{(1)} & 0 \\ \alpha_{13}^{(1)} & 0 & \alpha_{33}^{(1)} \end{pmatrix},$$
$$\alpha^{(2)} = \begin{pmatrix} 0 & 0 & \alpha_{13}^{(2)} \\ 0 & 0 & 0 \\ \alpha_{13}^{(2)} & 0 & \alpha_{33}^{(1)} \end{pmatrix}. \tag{12}$$

4.1.3. Orthorhombic system

There is only one Laue class, i.e. mmm_h $(2_h2_h2, mm2, 2_hmm_h$ and $mmm_h)$, and

$$\alpha^{(1)} = \begin{pmatrix} \alpha_{11}^{(1)} & 0 & 0 \\ 0 & \alpha_{22}^{(1)} & 0 \\ 0 & 0 & \alpha_{33}^{(1)} \end{pmatrix},$$
$$\alpha^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \alpha_{33}^{(1)} \end{pmatrix}. \tag{13}$$

4.1.4. Tetragonal, trigonal and hexagonal system

Discussing as stated above, we can obtain the matrix forms of thermal-expansion-coefficient tensors under the point groups of tetragonal system, trigonal

system and hexagonal system as follows:

$$\alpha^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \alpha_{33}^{(1)} \end{pmatrix},$$

$$\alpha^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \alpha_{33}^{(2)} \end{pmatrix}. \quad (14)$$

Now we have obtained all matrix forms of the thermal expansion coefficient tensors of 1D quasicrystals. From these matrices, we can see that the thermal expansion effects of 1D quasicrystals are affected not only by acoustic phonon strains and also by acoustic phason strains. This is very different from those of 2D quasicrystals discussed by Yang *et al.*[19] From this we can predict that the specific of heat of 1D quasicrystals should be related to the phason train in the complementary space.

4.2. The matrix forms of the piezoelectric coefficient tensors

4.2.1. Point group 1

Here, $d^{(1)}$ has 18 independent components, i.e.

$$d^{(1)} = \begin{pmatrix} d_{11}^{(1)} & d_{12}^{(1)} & d_{13}^{(1)} & d_{14}^{(1)} & d_{15}^{(1)} & d_{16}^{(1)} \\ d_{21}^{(1)} & d_{22}^{(1)} & d_{23}^{(1)} & d_{24}^{(1)} & d_{25}^{(1)} & d_{26}^{(1)} \\ d_{31}^{(1)} & d_{32}^{(1)} & d_{33}^{(1)} & d_{34}^{(1)} & d_{35}^{(1)} & d_{36}^{(1)} \end{pmatrix}, \quad (15)$$

and $d^{(2)}$ has nine independent components, i.e.

$$d^{(2)} = \begin{pmatrix} 0 & 0 & d_{13}^{(2)} & d_{14}^{(2)} & d_{15}^{(2)} & 0 \\ 0 & 0 & d_{23}^{(2)} & d_{24}^{(2)} & d_{25}^{(2)} & 0 \\ 0 & 0 & d_{33}^{(2)} & d_{34}^{(2)} & d_{35}^{(2)} & 0 \end{pmatrix}. \quad (16)$$

4.2.2. Point group 2

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{24}^{(1)} & d_{25}^{(1)} & 0 \\ d_{31}^{(1)} & d_{32}^{(1)} & d_{33}^{(1)} & 0 & 0 & d_{36}^{(1)} \end{pmatrix}, \quad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{24}^{(1)} & d_{25}^{(1)} & 0 \\ 0 & 0 & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}. \quad (17)$$

4.2.3. Point group m_h

$$d^{(1)} = \begin{pmatrix} d_{11}^{(1)} & d_{12}^{(1)} & d_{13}^{(1)} & 0 & 0 & d_{16}^{(1)} \\ d_{21}^{(1)} & d_{22}^{(1)} & d_{23}^{(1)} & 0 & 0 & d_{26}^{(1)} \\ 0 & 0 & 0 & d_{34}^{(1)} & d_{35}^{(1)} & 0 \end{pmatrix}, \quad d^{(2)} = \begin{pmatrix} 0 & 0 & d_{13}^{(2)} & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & d_{23}^{(2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{34}^{(2)} & d_{35}^{(2)} & 0 \end{pmatrix}. \quad (18)$$

4.2.4. Point group 2_h

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & 0 & d_{16}^{(1)} \\ d_{21}^{(1)} & d_{22}^{(1)} & d_{23}^{(1)} & 0 & d_{25}^{(1)} & 0 \\ 0 & 0 & 0 & d_{34}^{(1)} & 0 & d_{36}^{(1)} \end{pmatrix}, \quad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & d_{23}^{(2)} & 0 & d_{25}^{(2)} & 0 \\ 0 & 0 & 0 & d_{34}^{(2)} & 0 & 0 \end{pmatrix}. \quad (19)$$

4.2.5. Point group m

$$d^{(1)} = \begin{pmatrix} d_{11}^{(1)} & d_{12}^{(1)} & d_{13}^{(1)} & 0 & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{24}^{(1)} & 0 & d_{26}^{(1)} \\ d_{31}^{(1)} & d_{32}^{(1)} & d_{33}^{(1)} & 0 & d_{35}^{(1)} & 0 \end{pmatrix}, \quad d^{(2)} = \begin{pmatrix} 0 & 0 & d_{13}^{(2)} & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{24}^{(2)} & 0 & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & d_{35}^{(2)} & 0 \end{pmatrix}. \quad (20)$$

4.2.6. Point group 2_h2_h2

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{25}^{(1)} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{36}^{(1)} \end{pmatrix}, \quad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{25}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (21)$$

4.2.7. Point group $mm2$

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{24}^{(1)} & 0 & 0 \\ d_{31}^{(1)} & d_{32}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{24}^{(2)} & 0 & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{22}$$

4.2.8. Point group $2_h mm_h$

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & d_{16}^{(1)} \\ d_{21}^{(1)} & d_{22}^{(1)} & d_{23}^{(1)} & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{34}^{(1)} & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_{23}^{(2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{34}^{(2)} & 0 & 0 \end{pmatrix}. \tag{23}$$

4.2.9. Point group 4

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{15}^{(1)} & -d_{14}^{(1)} & 0 \\ d_{31}^{(1)} & d_{31}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & -d_{14}^{(2)} & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{24}$$

4.2.10. Point group $\bar{4}$

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & -d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{15}^{(1)} & d_{14}^{(1)} & 0 \\ d_{31}^{(1)} & -d_{31}^{(1)} & 0 & 0 & 0 & d_{36}^{(1)} \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & -d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & d_{14}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{25}$$

4.2.11. Point group 42_h2_h

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(1)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{26}$$

4.2.12. Point group $4mm$

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{15}^{(1)} & 0 & 0 \\ d_{31}^{(1)} & d_{31}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & 0 & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{27}$$

4.2.13. Point group $\bar{4}2_h m$

$$d^{(1)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14}^{(1)} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{36}^{(1)} \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{28}$$

4.2.14. Point group 3

$$d^{(1)}=\begin{pmatrix} d_{11}^{(1)} & -d_{11}^{(1)} & 0 & d_{14}^{(1)} & d_{15}^{(1)} & -2d_{22}^{(1)} \\ -d_{22}^{(1)} & d_{22}^{(1)} & 0 & d_{15}^{(1)} & -d_{14}^{(1)} & -2d_{11}^{(1)} \\ d_{31}^{(1)} & d_{31}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)}=\begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & -d_{14}^{(2)} & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{29}$$

4.2.15. Point group 32_h

$$d^{(1)} = \begin{pmatrix} d_{11}^{(1)} & -d_{11}^{(1)} & 0 & d_{14}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(1)} & -2d_{11}^{(1)} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{30}$$

4.2.16. Point group $3m$

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(1)} & -2d_{22}^{(1)} \\ -d_{22}^{(1)} & d_{22}^{(1)} & 0 & d_{15}^{(1)} & 0 & 0 \\ d_{31}^{(1)} & d_{31}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & 0 & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{31}$$

4.2.17. Point group 6

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{15}^{(1)} & -d_{14}^{(1)} & 0 \\ d_{31}^{(1)} & d_{31}^{(1)} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & -d_{14}^{(2)} & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{32}$$

4.2.18. Point group $\bar{6}$

$$d^{(1)} = \begin{pmatrix} d_{11}^{(1)} & -d_{11}^{(1)} & 0 & 0 & 0 & -2d_{22}^{(1)} \\ -d_{22}^{(1)} & d_{22}^{(1)} & 0 & 0 & 0 & -2d_{11}^{(1)} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = 0. \tag{33}$$

4.2.19. Point group 62_h2_h

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(1)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & d_{14}^{(2)} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14}^{(2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{34}$$

4.2.20. Point group $6mm$

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(1)} & 0 \\ 0 & 0 & 0 & d_{15}^{(1)} & 0 & 0 \\ d_{31}^{(1)} & d_{31} & d_{33}^{(1)} & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 & d_{15}^{(2)} & 0 \\ 0 & 0 & 0 & d_{15}^{(2)} & 0 & 0 \\ 0 & 0 & d_{33}^{(2)} & 0 & 0 & 0 \end{pmatrix}. \tag{35}$$

4.2.21. Point group $\bar{6}m2_h$

$$d^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -2d_{22}^{(1)} \\ -d_{22}^{(1)} & d_{22}^{(1)} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \qquad d^{(2)} = 0. \tag{36}$$

4.2.22. Point groups $\bar{1}$, $\bar{2}$, $2/m_h$, $2_h/m$, mmm_h, $4/m_h$, $4/m_hmm$, $\bar{3}$, $6/m_h$, $6/mmm_h$

$$d^{(1)} = 0, \qquad d^{(2)} = 0. \tag{37}$$

So far, we have obtained the matrix forms of the piezoelectric coefficient tensors under 31 point-groups of 1D quasicrystals. Among these matrices, most of $d^{(1)}$ are the same as those of 3D periodic crystals;

however since 2 and 2_h, m and m_h are different point groups, $d^{(1)}$ with these point group symmetries have different matrix forms, i.e. $d_2^{(1)} \neq d_{2_h}^{(1)}$ and $d_m^{(1)} \neq d_{m_h}^{(1)}$. In addition, if $d^{(1)}$=0, then $d^{(2)}$ is equal to zero. This means that a 1D quasicrystal with centro-symmetry definitively has no piezoelectric effect.

5. Summary

In this paper, using group representation, we have derived the character formulae of representation matrices for physical property tensors of 1D quasicrystals. Based on the formulae, we have computed the numbers of independent components of these physical property tensors and listed them in Table 1. In addition, starting from the generated matrices of point groups and using the Neumann theorem, we have deduced the matrix forms of thermal-expansion coefficient and piezoelectric coefficient tensors under the 31 point groups of 1D quasicrystals. This is an important complement of the quasicrystal physical property. Analysing these matrices, we can see that the thermal expansion effects of 1D quasicrystals are affected not only by acoustic phonon strains but also by phason strains, which implies that both phonon and phason strains are changed with temperature in the vicinity of the equilibrium state. This is quite different from the case of 2D quasicrystals discussed by Yang *et al.*[19] From this point we can also predict that the specific of heat of 1D quasicrystals should be related to the phason train in the complementary space.[21–23] Moreover, if the piezoelectric coefficients $d^{(1)} = 0$, then $d^{(2)}$ is equal to zero. Thus, the 1D quasicrystals with centro-symmetry do not have piezoelectric effects.

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