Elastic strains induced by electric fields in quasicrystals

1995 J. Phys.: Condens. Matter 7 L499

(http://iopscience.iop.org/0953-8984/7/39/001)

J. Phys.: Condens. Matter 7 (1995) L499–L502. Printed in the UK

LETTER TO THE EDITOR

Elastic strains induced by electric fields in quasicrystals

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

Received 5 July 1995

Abstract. The classical formulae of piezoelectric and electrostriction effects in crystals are generalized to quasicrystals. Two types of strain (phonon strain and phason strain) induced by electric fields have been studied. According to group representation theory, the matrix forms of piezoelectric and electrostriction tensors of two-dimensional pentagonal, octagonal, decagonal, dodecagonal and three-dimensional icosahedral cubic quasicrystals are given. If one takes the external field as a magnetic field, these tensors can also be used to describe magnetoelastic effects in quasicrystals.

As is well known, the extensive usage of piezoelectric crystals has made a great change in this world [1]. The elasticity theory [2–5] and the electronic structure and electric transport [6] of quasicrystals have been studied separately. In our recent paper about the thermodynamics of equilibrium properties of quasicrystals [7], we discussed the piezoelectric effect in quasicrystals and found that many types of quasicrystal do not possess a piezoelectric effect. However, the higher-order effects, i.e. electrostriction effects, can also have a great effect in this case. In this short letter, we will discuss the piezoelectric and electrostriction effects in quasicrystals. By the group representation theory, we have given the standard methods to calculate the numbers and invariants of independent constants of physical property tensors in quasicrystals [8, 9]. Using these methods, we can give the matrix forms of piezoelectric and electrostrictional tensors for two-dimensional (2D) pentagonal, octagonal, decagonal, dodecagonal and three-dimensional (3D) icosahedral cubic quasicrystals (QCs).

As we know, the most important difference in the elastic properties between crystals and quasicrystals is that there are two kinds of elastic displacement field in quasicrystals: the phonon displacement $\boldsymbol{u}$ and the phason displacement $\boldsymbol{w}$. Correspondingly, there are two kinds of strain field: $E_{ij} = \frac{1}{2}(\partial_j u_i + \partial_i u_j)$ and $W_{ij} = \partial_j w_i$, and two kinds of stress field: T_{ij} and H_{ij} [4, 5]. Obviously, these characteristics will have an influence on the thermodynamics of quasicrystals. In [7], we suggested the thermodynamics of equilibrium properties of QCs. The linear relations between thermal, electrical, magnetic and mechanical properties were discussed there. In [7], we chose stresses T_{ij}, H_{ij}, electrical or magnetic field intensity F_i and absolute temperature θ as a set of independent variables, strains E_{ij}, W_{ij}, electric displacement or magnetic induction vector D_i and entropy S as a set of dependent variables and Gibbs free energy function G

$$G = U - T_{ij}E_{ij} - H_{ij}W_{ij} - F_iD_i - \theta S \tag{1}$$

† Address for correspondence: Professor Di-hua Ding, Department of Physics, Wuhan University, 430072 Wuhan, People's Republic of China.

0953-8984/95/390499+04$19.50

as the state function, where U is the internal energy of the system. The increase in U can be expressed as

$$dU = T_{ij}\,dE_{ij} + H_{ij}\,dW_{ij} + F_i\,dD_i + \theta\,dS$$

by the first and second laws of thermodynamics, so

$$dG = -E_{ij}\,dT_{ij} - W_{ij}\,dH_{ij} - D_i\,dF_i - S\,d\theta. \tag{2}$$

In isothermal conditions, the electric displacement produced by stresses (isothermal direct piezoelectric effect) is given by

$$\begin{aligned} dD_i &= \left(\frac{\partial D_i}{\partial T_{jk}}\right)_{H,F,\theta} dT_{jk} + \left(\frac{\partial D_i}{\partial H_{jk}}\right)_{T,F,\theta} dH_{jk} = -\left(\frac{\partial^2 G}{\partial F_i \partial T_{jk}}\right)_\theta dT_{jk} - \left(\frac{\partial^2 G}{\partial F_i \partial H_{jk}}\right)_\theta dH_{jk} \\ &= d^{(1)}_{ijk}\,dT_{jk} + d^{(2)}_{ijk}\,dH_{jk}. \end{aligned} \tag{3}$$

For the converse process, the elastic strains produced by an electric field (isothermal converse piezoelectric effect) are

$$\begin{aligned} dE_{ij} &= \left(\frac{\partial E_{ij}}{\partial F_k}\right)_{T,H,\theta} dF_k = -\left(\frac{\partial^2 G}{\partial T_{ij}\partial F_k}\right)_\theta dF_k = \underline{d}^{(1)}_{ijk}\,dF_k \\ dW_{ij} &= \left(\frac{\partial W_{ij}}{\partial F_k}\right)_{T,H,\theta} dF_k = -\left(\frac{\partial^2 G}{\partial H_{ij}\partial F_k}\right)_\theta dF_k = \underline{d}^{(2)}_{ijk}\,dF_k. \end{aligned} \tag{4}$$

The coefficients $d^{(1)}$, $d^{(2)}$, $\underline{d}^{(1)}$, $\underline{d}^{(2)}$ in equations (3) and (4) are called piezoelectric tensors (rank three). Since G is a state function, the order of differentiation is immaterial; one can obtain

$$d^{(1)}_{ijk} = \underline{d}^{(1)}_{jki} \qquad d^{(2)}_{ijk} = \underline{d}^{(2)}_{jki}. \tag{5}$$

We have calculated the third-rank tensors $d^{(1)}$ and $d^{(2)}$ for twenty-six 2D QCs (pentagonal, octagonal, decagonal and dodecagonal QCs) and three 3D QCs (icosahedral 235, $m\overline{35}$ and cubic 432 QCs), and found that only twelve QCs, i.e., those which possess point groups N, $N2$ (or $N22$), Nm (or Nmm), $N = 5, 8, 10, 12$, have non-zero components in $d^{(1)}_{ijk}$ and three pentagonal QCs, i.e., 5, 52, $5m$, have non-zero components in $d^{(2)}_{ijk}$. Like conventional crystals, when there are no piezoelectric effects due to symmetry of the solid, the strain induced by electric field is characterized by the electrostriction effect.

In order to consider the electrostriction effect, equation (4) should be rewritten as

$$\begin{aligned} dE_{ij} &= \left(\frac{\partial E_{ij}}{\partial F_k}\right)_{T,H,\theta} dF_k + Q^{(1)}_{klij}\,dF_k\,dF_l \\ dW_{ij} &= \left(\frac{\partial W_{ij}}{\partial F_k}\right)_{T,H,\theta} dF_k + Q^{(2)}_{klij}\,dF_k\,dF_l \end{aligned} \tag{6}$$

where

$$\begin{aligned} Q^{(1)}_{klij} &= \left(\frac{\partial^2 E_{ij}}{\partial F_k \partial F_l}\right)_{T,H,\theta} = -\left(\frac{\partial^3 G}{\partial T_{ij}\partial F_k \partial F_l}\right)_\theta \\ Q^{(2)}_{klij} &= \left(\frac{\partial^2 W_{ij}}{\partial F_k \partial F_l}\right)_{T,H,\theta} = -\left(\frac{\partial^3 G}{\partial H_{ij}\partial F_k \partial F_l}\right)_\theta \end{aligned} \tag{7}$$

are electrostriction tensors which are used to describe respectively the phonon strain and phason strain changed by quadratic effects of electric field. One can see that the first equation in equation (6) is the same as for conventional crystals and such an effect may exist in solids in any symmetry.

In [8], we classified the physical properties of tensors of QCs by group representation theory. Taking the same conventions as there, vectors in physical subspace transform under the representation Γ_A (3D representation), whereas vectors in complementary subspace transform under another representation Γ_b (3D representation for 3D QCs, 2D representation for 2D QCs), and the notation {} means that the symmetric part in {} is chosen.

From the definition of $d^{(1)}$, $d^{(2)}$, $Q^{(1)}$, $Q^{(2)}$, we can analyse the internal symmetries and obtain the matrix forms for every kind of QC. Both phonon strain E_{ij} and stress T_{ij} exist in physical subspace, and the subscripts i and j can commute with each other; but for phason strain W_{ij} and stress H_{ij} the subscripts i and j are in complementary and physical subspace, respectively; the electric field vector always exists in physical subspace. So, the tensors $d^{(1)}$, $d^{(2)}$, $Q^{(1)}$ and $Q^{(2)}$ transform under $\Gamma_A \times \{\Gamma_A \times \Gamma_A\}$, $\Gamma_A \times (\Gamma_A \times \Gamma_B)$, $\{\Gamma_A \times \Gamma_A\} \times \{\Gamma_A \times \Gamma_A\}$ and $\{\Gamma_A \times \Gamma_A\} \times (\Gamma_A \times \Gamma_B)$, respectively.

Table 1. The forms of electrostriction coefficient tensors $Q^{(1)}_{klij}$ ($Q^{(1)}_{klij}$ are arranged as $kl = 11$, 22, 33, 23, 31, 12, $ij = 11$, 22, 33, 23, 31, 12 as in the case of crystals [1]).

235, $m\overline{3}\overline{5}$

$$\begin{bmatrix} Q_1 & Q_2 & Q_2 & 0 & 0 & 0 \\ Q_2 & Q_1 & Q_2 & 0 & 0 & 0 \\ Q_2 & Q_2 & Q_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & (Q_1-Q_2)/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & (Q_1-Q_2)/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & (Q_1-Q_2)/2 \end{bmatrix}$$

(2)

432 (CQC)

$$\begin{bmatrix} Q_1 & Q_2 & Q_2 & 0 & 0 & 0 \\ Q_2 & Q_1 & Q_2 & 0 & 0 & 0 \\ Q_2 & Q_2 & Q_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & Q_3 \end{bmatrix}$$

(3)

5, $\overline{5}$, N, $\overline{N}$, N/m ($N = 8, 10, 12$)

$$\begin{bmatrix} Q_1 & Q_2 & Q_3 & 0 & 0 & -Q_8 \\ Q_2 & Q_1 & Q_3 & 0 & 0 & Q_8 \\ Q_5 & Q_5 & Q_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_6 & -Q_7 & 0 \\ 0 & 0 & 0 & Q_7 & Q_6 & 0 \\ Q_8 & -Q_8 & 0 & 0 & 0 & (Q_1-Q_2)/2 \end{bmatrix}$$

(8)

$5m$, 52, $\overline{5}m$, Nmm, $N22$, $\overline{N}m2$, N/mmm ($N = 8$, 10, 12)

$$\begin{bmatrix} Q_1 & Q_2 & Q_3 & 0 & 0 & 0 \\ Q_2 & Q_1 & Q_3 & 0 & 0 & 0 \\ Q_5 & Q_5 & Q_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & Q_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & (Q_1-Q_2)/2 \end{bmatrix}$$

(6)

We have already given the matrix forms $d^{(1)}$, $d^{(2)}$ for all kinds of QC with non-crystallographic symmetries and cubic QC (CQC) in [7]. Among $d^{(1)}_{kij}$ there are four independent non-vanishing components $d^{(1)}_{123} = -d^{(1)}_{231}$, $d^{(1)}_{131} = d^{(1)}_{223}$, $d^{(1)}_{311} = d^{(1)}_{322}$ and $d^{(1)}_{333}$ for the point groups N, one independent component $d^{(1)}_{123} = -d^{(1)}_{231}$ for $N2$ or $N22$ and three independent components $d^{(1)}_{131} = d^{(1)}_{223}$, $d^{(1)}_{311} = d^{(1)}_{322}$, $d^{(1)}_{333}$ for Nm or Nmm symmetries, respectively, where $N = 5$, 8, 10, 12. Among $d^{(2)}_{kij}$, there are two independent components ($-d^{(2)}_{111} = d^{(2)}_{122} = d^{(2)}_{212} = d^{(2)}_{221}$, $d^{(2)}_{112} = d^{(2)}_{121} = d^{(2)}_{211} = -d^{(2)}_{222}$) for the point group 5, one independent ($-d^{(2)}_{111} = d^{(2)}_{122} = d^{(2)}_{212} = d^{(2)}_{221}$) for 52 and one independent ($d^{(2)}_{112} = d^{(2)}_{121} = d^{(2)}_{211} = -d^{(2)}_{222}$) for $5m$ symmetry, respectively. For the other symmetries, $d^{(1)}_{kij} = 0$, $d^{(2)}_{kij} = 0$. The forms of the electrostriction coefficient tensors are listed in tables 1 and 2, where the number in parentheses under each coefficient matrix is the number of independent constants. From the results, one can see that none of the dodecagonal QCs

Table 2. The forms of electrostriction coefficient tensors $Q^{(2)}_{klij}$ ($Q^{(2)}_{klij}$ are arranged as $kl = 11, 22, 33, 23, 31, 12$, $ij = 11, 22, 33, 12, 13, 21, 23, 31, 32$ and $11, 22, 12, 13, 21, 23$ for 3D QCs (IQC, CQC) and 2D QCs (pentagonal, octagonal, decagonal and dodecagonal QCs), respectively).

235, $m\overline{3}\overline{5}$

$$S\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & -1 \\ 1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 \end{bmatrix} \quad (1)$$

432 (CQC)

$$\begin{bmatrix} S_1 & S_2 & S_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ S_2 & S_1 & S_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ S_2 & S_2 & S_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & S_3 & 0 & 0 & S_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & S_3 & 0 & 0 & S_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & S_3 & 0 & 0 & S_3 \end{bmatrix} \quad (3)$$

2D quasicrystals

$$\begin{bmatrix} S_1 & S_1 & -S_2 & S_3 & S_2 & S_4 \\ -S_1 & -S_1 & S_2 & -S_3 & -S_2 & -S_4 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ S_6 & -S_6 & -S_5 & 0 & -S_5 & 0 \\ S_5 & -S_5 & S_6 & 0 & S_6 & 0 \\ -S_2 & -S_2 & -S_1 & S_4 & S_1 & -S_3 \end{bmatrix}$$

for $\overline{5}$ Laue class $S_1, S_2, S_3, S_4, S_5, S_6 \neq 0$;
for $\overline{5}m$ Laue class $S_2 = S_3 = S_5 = 0$;
for $8/m$ or $10/m$ Laue class $S_3 = S_4 = S_5 = S_6 = 0$;
for $8/mmm$ or $10/mmm$ Laue class $S_2 = S_3 = S_4 = S_5 = S_6 = 0$;
for $12/m$ or $12/mmm$ Laue class $Q^{(2)}_{klij} = 0$

possess the phason strain part of the electrostriction which is just the same as having no coupling term between phonon strain and phason strain the in linear elastic energy in these structures [10]. In particular, for a 2D QC with $\overline{12}$, $12/m$, $\overline{12}m2$ or $12/mmm$, $d^{(2)}_{ijk} = 0$, $Q^{(2)}_{klij} = 0$, i.e., phason strains are not changed by an electric field up to quadratic order. If one takes the external field as a magnetic field, the above tensors can also be used to describe magnetoelastic effects in quasicrystals. The study of unified non-linear thermodynamics in quasicrystals is in progress.

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

References

[1] Cady W G 1946 *Piezoelectricity* (New York: McGraw-Hill)
[2] Levine D, Lubensky T C, Ostlund S, Ramaswamy S, Steinhardt P J and Toner J 1985 *Phys. Rev. Lett.* **54** 1520
[3] Socolar J E S 1989 *Phys. Rev.* B **39** 10 519
[4] Yang W G, Wang R, Ding D H and Hu C Z 1993 *Phys. Rev.* B **48** 6999
[5] Ding D H, Yang W G, Hu C Z and Wang R 1993 *Phys. Rev.* B **48** 7003
[6] Fujiwara T, Laissardiere G T and Yamamoto S 1994 *Mater. Sci. Forum* **150–151** 387
[7] Yang W G, Ding D H, Wang R and Hu C Z 1995 *Z. Phys.* B at press
[8] Yang W G, Ding D H, Hu C Z and Wang R 1994 *Phys. Rev.* B **49** 12 656
[9] Yang W G, Wang R, Ding D H and Hu C Z 1995 *J. Phys.: Condens. Matter* **7** 7099
[10] Yang W G, Lei J L, Ding D H, Wang R and Hu C Z 1995 *Phys. Lett.* **200A** 177