# SHORT COMMUNICATIONS

*Acta Cryst.* (1999). A**55**, 558–560

## Positive-definite conditions of elastic constants of two-dimensional quasicrystals with noncrystallographic symmetries†

Jianbo Wang, Ruikang Zhang, Di-Hua Ding and Renhui Wang* *at Department of Physics, Wuhan University, Wuhan 430072, People's Republic of China. E-mail: rhwang@image.blem.ac.cn*

(*Received 30 June 1998; accepted 26 August 1998*)

### Abstract

In the present work, the positive-definite conditions of the elastic constants of two-dimensional (2D) quasicrystals with non-crystallographic symmetries have been derived. These results are necessary for studying elastic and mechanical properties of two-dimensional quasicrystals both in theory and in experiment.

### 1. Introduction

Since the first quasicrystal structure was observed, great progress has been made in the study of the elastic properties of quasicrystals. The independent elastic constants and the elastic energy have already been derived for pentagonal planar quasiperiodic structure and icosahedral phase (Levine *et al.*, 1985; Lubensky *et al.*, 1985) and for planar quasicrystals with eight-, ten- and twelvefold symmetries (Socolar, 1989), on the basis of representation theory. In addition, the positive-definite conditions satisfied by the elastic constants have already been given for an icosahedral quasicrystal (Jaric & Nelson, 1988; Ishii, 1992).

It is well known that a two-dimensional quasicrystal (2D QC) refers not to a real plane but to a three-dimensional solid with two-dimensional quasiperiodic and one-dimensional periodic structure. According to Janssen's treatment (Janssen, 1992), Hu *et al.* (1996) have discussed the point groups of all 2D QCs in detail. Their work shows that there are 10 systems, 18 Laue classes and 57 point groups. Among them, 6 systems, 10 Laue classes and 31 point groups are crystallographically allowable (called the first kind), and the remaining 4 systems, 8 Laue classes and 26 point groups are crystallographically forbidden (called the second kind). In addition, using group-representation theory, they have also calculated the numbers of independent elastic constants, the scalar invariants of the strain tensors up to second order (Hu *et al.*, 1996) and the concrete matrix forms of the elastic constants (Hu *et al.*, 1997) for all 2D QCs with Fourier module of rank 5.

The requirement that the strain energy of a crystal must be positive poses further restrictions on the elastic constants. Nye (1957) discussed positive-definite conditions of the elastic constants of crystals. In the present work, we wish to deduce the positive-definite conditions of all elastic constants for the second kind of 2D QCs mentioned above. It is clear that the results given here are necessary for studying elastic and mechanical properties of 2D QCs both in theory and in experiment.

† Project supported by the National Natural Science Foundation of China.

### 2. Elastic constants of two-dimensional quasicrystals with non-crystallographic symmetries

According to Hu *et al.* (1996, 1997), the number of elastic constants related to the phonon field is the same for all two-dimensional quasicrystals (Table 1), which is the same as that for the crystalline hexagonal system. The elastic constants related to the phason field and the phonon–phason coupling are listed below sorted by Laue class.

(I) Laue class 11 (point group: 5, $\bar{5}$)

The elastic constants $K_{ijkl}$ related to the phason field are listed in Table 2, and $R_{ijkl}$ the phonon–phason coupling in Table 3.

(II) Laue class 12 (point group: $5m$, 52, $\bar{5}m$)

If $2 \parallel x_1$, $m \perp x_1$, then $K_6 = R_2 = R_3 = R_5 = 0$ in Tables 2 and 3.

If $2 \parallel x_2$, $m \perp x_2$, then $K_7 = R_2 = R_4 = R_6 = 0$ in Tables 2 and 3.

(III) Laue class 13 (point group: 10, $\overline{10}$, $10/m$)

$K_6 = K_7 = R_3 = R_4 = R_5 = R_6 = 0$ in Tables 2 and 3.

(IV) Laue class 14 (point group: $10mm$, 1022, $\overline{10}m2$, $10/mmm$)

$K_6 = K_7 = R_2 = R_3 = R_4 = R_5 = R_6 = 0$ in Tables 2 and 3.

(V) Laue class 15 (point group: 8, $\bar{8}$, $8/m$)

The elastic constants related to the phason field are listed in Table 4, and the phonon–phason coupling in Table 5.

(VI) Laue class 16 (point group: $8mm$, 822, $\bar{8}m2$, $8/mmm$)

$K_5 = R_2 = 0$ in Tables 4 and 5.

(VII) Laue class 17 (point group: 12, $\overline{12}$, $12/m$)

The elastic constants related to the phason field are the same as those of Laue class 15, *i.e.* Table 4, and all the elastic constants of the phonon–phason coupling are zero.

(VIII) Laue class 18 (point group: $12mm$, 1222, $\overline{12}m2$, $12/mmm$)

The elastic constants related to the phason field are the same as those of Laue class 16, and all the elastic constants of the phonon–phason coupling are zero.

According to the generalized linear elasticity theory of quasicrystals (Ding *et al.*, 1993), we may write the elastic energy density of two-dimensional quasicrystals as

$$F = \tfrac{1}{2}C_{ijkl}E_{ij}E_{kl} + \tfrac{1}{2}K_{ijkl}W_{ij}W_{kl} + R_{ijkl}E_{ij}W_{kl} = \tfrac{1}{2}\begin{bmatrix} E & W \end{bmatrix}\begin{bmatrix} [C] & [R] \\ [R]^T & [K] \end{bmatrix}\begin{bmatrix} E \\ W \end{bmatrix} \quad (i,j,k,l = 1,2,3), \qquad (1)$$

where $[C]$ denotes a $9 \times 9$ elastic constant matrix consisting of $C_{ijkl}$ related to the phonon field, $[K]$ denotes a $6 \times 6$ elastic constant matrix related to the phason field with matrix

Table 1. *The elastic constants ($C_{ijkl}$) related to the phonon field of two-dimensional quasicrystals*

The numbers in column 1 are subscripts *ij*, and those in row 1 are subscripts *kl*.

| | 11 | 22 | 33 | 23 | 31 | 12 |
|---|---|---|---|---|---|---|
| 11 | $C_{11}$ | $C_{12}$ | $C_{13}$ | 0 | 0 | 0 |
| 22 | $C_{12}$ | $C_{11}$ | $C_{13}$ | 0 | 0 | 0 |
| 33 | $C_{13}$ | $C_{13}$ | $C_{33}$ | 0 | 0 | 0 |
| 23 | 0 | 0 | 0 | $C_{44}$ | 0 | 0 |
| 31 | 0 | 0 | 0 | 0 | $C_{44}$ | 0 |
| 12 | 0 | 0 | 0 | 0 | 0 | $C_{66}$† |

† Where $C_{66} = (C_{11} - C_{12})/2$.

elements $K_{ijkl}$, $[R]$ is a $9 \times 6$ elastic constant matrix related to the phonon–phason coupling with matrix elements $R_{ijkl}$, and $[R]^T$ is the transpose matrix of $[R]$. $E$ and $W$ denote the phonon and phason strain fields consisting of $E_{ij}$ and $W_{ij}$, respectively.

In order that this energy density is greater than zero for all strain values unless all the strain values are zero, *i.e.* the quadratic form (1) must be positive-definite, the following conditions are required:

$$C_{1111} > 0, \quad \begin{vmatrix} C_{1111} & C_{1122} \\ C_{2211} & C_{2222} \end{vmatrix} > 0, \cdots,$$

$$\begin{vmatrix} C_{1111} & C_{1122} & \cdots & C_{1121} & R_{1111} & \cdots & R_{1113} \\ C_{2211} & C_{2222} & \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_{2111} & \cdots & \cdots & C_{2121} & R_{2111} & \cdots & R_{2113} \\ R_{1111} & \cdots & \cdots & R_{2111} & K_{1111} & \cdots & K_{1113} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ R_{1113} & \cdots & \cdots & R_{2113} & K_{1311} & \cdots & K_{1313} \end{vmatrix} > 0,$$

$$\begin{vmatrix} C_{1111} & C_{1122} & \cdots & C_{1121} & R_{1111} & \cdots & R_{1113} & R_{1121} \\ C_{2211} & C_{2222} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_{2111} & \cdots & \cdots & C_{2121} & R_{2111} & \cdots & R_{2113} & R_{2121} \\ R_{1111} & \cdots & \cdots & R_{2111} & K_{1111} & \cdots & K_{1113} & K_{1121} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ R_{1113} & \cdots & \cdots & R_{2113} & K_{1311} & \cdots & K_{1313} & K_{1321} \\ R_{1121} & \cdots & \cdots & R_{2121} & K_{2111} & \cdots & K_{2113} & K_{2121} \end{vmatrix} > 0. \tag{2}$$

Applying the above conditions, we can deduce the restraint relations satisfied by the elastic constants.

### 3. Positive-definite conditions of elastic constants of non-crystallographic two-dimensional quasicrystals

Substituting the elastic constants of Laue classes 11–18 into the conditions described by (2), we derived the following results:

(I) The conditions of the elastic constants related to the phonon field are the same for all the Laue classes 11–18. The results are:

Table 2. *The elastic constants ($K_{ijkl}$) related to the phason field of Laue class 11*

The numbers in column 1 are subscripts *ij*, and those in row 1 are subscripts *kl*.

| | 11 | 22 | 23 | 12 | 13 | 21 |
|---|---|---|---|---|---|---|
| 11 | $K_1$ | $K_2$ | $K_7$ | 0 | $K_6$ | 0 |
| 22 | $K_2$ | $K_1$ | $K_7$ | 0 | $K_6$ | 0 |
| 23 | $K_7$ | $K_7$ | $K_4$ | $K_6$ | 0 | $-K_6$ |
| 12 | 0 | 0 | $K_6$ | $K_1$ | $-K_7$ | $-K_2$ |
| 13 | $K_6$ | $K_6$ | 0 | $-K_7$ | $K_4$ | $K_7$ |
| 21 | 0 | 0 | $-K_6$ | $-K_2$ | $K_7$ | $K_1$ |

Table 3. *The elastic constants ($R_{ijkl}$) related to the phonon–phason coupling of Laue class 11*

The numbers in column 1 are subscripts *ij*, related to the phonon field, and those in row 1 are subscripts *kl*, related to the phason field.

| | 11 | 22 | 23 | 12 | 13 | 21 |
|---|---|---|---|---|---|---|
| 11 | $R_1$ | $R_1$ | $R_6$ | $R_2$ | $R_5$ | $-R_2$ |
| 22 | $-R_1$ | $-R_1$ | $-R_6$ | $-R_2$ | $-R_5$ | $R_2$ |
| 33 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | $R_4$ | $-R_4$ | 0 | $R_3$ | 0 | $R_3$ |
| 31 | $-R_3$ | $R_3$ | 0 | $R_4$ | 0 | $R_4$ |
| 12 | $R_2$ | $R_2$ | $-R_5$ | $-R_1$ | $R_6$ | $R_1$ |

$$C_{44} > 0, \quad C_{11} > |C_{12}|, \quad (C_{11} + C_{12})C_{33} > 2C_{13}^2, \tag{3}$$

which are the same as those for hexagonal crystals (Nye, 1957).

(II) The other conditions are described as follows, sorted into Laue classes:

(*a*) Laue class 11

$$(K_1 - K_2)C_{44} > 2(R_3^2 + R_4^2) \tag{4}$$

$$(K_1 + K_2)(C_{11} - C_{12}) > 4(R_1^2 + R_2^2) \tag{5}$$

$$\begin{aligned}&(C_{11} - C_{12})(K_1 + K_2)K_4 - 2(C_{11} - C_{12})(K_6^2 + K_7^2) \\ &\quad - 4K_4(R_1^2 + R_2^2) + 8[K_6(R_1R_5 + R_2R_6) \\ &\quad + K_7(R_1R_6 - R_2R_5)] - 2(K_1 + K_2)(R_5^2 + R_6^2) > 0\end{aligned} \tag{6}$$

$$\begin{aligned}&(C_{11} - C_{12})C_{44}K_1K_4 - (C_{11} - C_{12})C_{44}(K_6^2 + K_7^2) \\ &\quad - 2C_{44}K_4(R_1^2 + R_2^2) - (C_{11} - C_{12})K_4(R_3^2 + R_4^2) \\ &\quad + 4C_{44}[K_6(R_1R_5 + R_2R_6) + K_7(R_1R_6 - R_2R_5)] \\ &\quad - 2C_{44}K_1(R_5^2 + R_6^2) + 2(R_3^2 + R_4^2)(R_5^2 + R_6^2) > 0\end{aligned} \tag{7}$$

$$\begin{aligned}&(C_{11} - C_{12})^2(K_1 + K_2)K_4 + 8K_7(C_{11} - C_{12})(R_1R_6 - R_2R_5) \\ &\quad - 2(C_{11} - C_{12})^2K_7^2 - 4(C_{11} - C_{12})K_4(R_1^2 + R_2^2) \\ &\quad - 2(C_{11} - C_{12})(K_1 + K_2)(R_5^2 + R_6^2) \\ &\quad + 8(R_1R_5 + R_2R_6)^2 > 0.\end{aligned} \tag{8}$$

One can prove that conditions (7) and (8) may be deduced from conditions (3)–(6). Therefore, the fundamental positive-definite conditions of elastic constants of Laue class 11 are (3)–(6). In the following, we list only the fundamental positive-definite conditions.

(*b*) Laue class 12

If $2 \parallel x_1$, $m \perp x_1$, then

Table 4. *The elastic constants ($K_{ijkl}$) related to the phason field of Laue class 15*

The numbers in column 1 are subscripts *ij*, and those in row 1 are subscripts *kl*.

| | 11 | 22 | 23 | 12 | 13 | 21 |
|---|---|---|---|---|---|---|
| 11 | $K_1$ | $K_2$ | 0 | $K_5$ | 0 | $K_5$ |
| 22 | $K_2$ | $K_1$ | 0 | $-K_5$ | 0 | $-K_5$ |
| 23 | 0 | 0 | $K_4$ | 0 | 0 | 0 |
| 12 | $K_5$ | $-K_5$ | 0 | $\Sigma$† | 0 | $K_3$ |
| 13 | 0 | 0 | 0 | 0 | $K_4$ | 0 |
| 21 | $K_5$ | $-K_5$ | 0 | $K_3$ | 0 | $\Sigma$† |

† Where $\Sigma = K_1 + K_2 + K_3$.

$$(K_1 - K_2)C_{44} > 2R_4^2, \quad (K_1 + K_2)(C_{11} - C_{12}) > 4R_1^2,$$
$$(C_{11} - C_{12})(K_1 + K_2)K_4 - 2(C_{11} - C_{12})K_7^2 - 4K_4R_1^2 + 8K_7R_1R_6 - 2(K_1 + K_2)R_6^2 > 0.$$

The above conditions can also be derived from the results of Laue class 11 by putting $K_6 = R_2 = R_3 = R_5 = 0$.

If $2 \parallel x_2$, $m \perp x_2$, then

$$(K_1 - K_2)C_{44} > 2R_3^2, \quad (K_1 + K_2)(C_{11} - C_{12}) > 4R_1^2,$$
$$(C_{11} - C_{12})(K_1 + K_2)K_4 - 2(C_{11} - C_{12})K_6^2 - 4K_4R_1^2 + 8K_6R_1R_5 - 2(K_1 + K_2)R_5^2 > 0.$$

The above conditions can also be derived from the results of Laue class 11 by putting $K_7 = R_2 = R_4 = R_6 = 0$.

(*c*) Laue class 13

$$K_1 - K_2 > 0, \quad K_4 > 0$$
$$(K_1 + K_2)(C_{11} - C_{12}) > 4(R_1^2 + R_2^2).$$

The above conditions can also be derived from the results of Laue class 11 by putting $K_6 = K_7 = R_3 = R_4 = R_5 = R_6 = 0$.

(*d*) Laue class 14

$$K_1 - K_2 > 0, \quad (K_1 + K_2)(C_{11} - C_{12}) > 4R_1^2, \quad K_4 > 0.$$

The above conditions can also be derived from the results of Laue class 13 by putting $R_2 = 0$.

(*e*) Laue class 15

$$K_1 - K_2 > 0, \quad (K_1 + K_2)(C_{11} - C_{12}) > 4(R_1^2 + R_2^2),$$
$$K_4 > 0, \quad (K_1 + K_2 + 2K_3)(K_1 - K_2) > 4K_5^2.$$

(*f*) Laue class 16

$$K_1 - K_2 > 0, \quad (K_1 + K_2)(C_{11} - C_{12}) > 4R_1^2,$$
$$K_4 > 0, \quad K_1 + K_2 + 2K_3 > 0.$$

Table 5. *The elastic constants ($R_{ijkl}$) related to the phonon–phason coupling of Laue class 15*

The numbers in column 1 are subscripts *ij*, related to the phonon field, and those in row 1 are subscripts *kl*, related to the phason field.

| | 11 | 22 | 23 | 12 | 13 | 21 |
|---|---|---|---|---|---|---|
| 11 | $R_1$ | $R_1$ | 0 | $R_2$ | 0 | $-R_2$ |
| 22 | $-R_1$ | $-R_1$ | 0 | $-R_2$ | 0 | $R_2$ |
| 33 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 0 | 0 | 0 | 0 | 0 | 0 |
| 31 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | $R_2$ | $R_2$ | 0 | $-R_1$ | 0 | $R_1$ |

The above conditions can also be derived from the results of Laue class 15 by putting $K_5 = R_2 = 0$.

(*g*) Laue class 17

$$K_1 > |K_2|, \quad K_4 > 0, \quad (K_1 + K_2 + 2K_3)(K_1 - K_2) > 4K_5^2.$$

The above conditions can also be derived from the results of Laue class 15 by putting all $R = 0$.

(*h*) Laue class 18

$$K_1 > |K_2|, \quad K_4 > 0, \quad K_1 + K_2 + 2K_3 > 0.$$

The above conditions can also be derived from the results of Laue class 16 by putting all $R = 0$.

## References


Ding, D. H., Yang, W. G., Hu, C. Z. & Wang, R. (1993). *Phys. Rev.B*, **48**, 7003–7010.

Hu, C. Z., Wang, R., Yang, W. G. & Ding, D. H. (1996). *Acta Cryst.* A**52**, 251–256.

Hu, C. Z., Yang, W. G., Wang, R. & Ding, D. H. (1997). *Prog. Phys.* **17**, 345–375. (In Chinese.)

Ishii, Y. (1992). *Phys. Rev. B*, **45**, 5228–5239.

Janssen, T. (1992). *Z. Kristallogr.* **198**, 17–32.

Jaric, M. V. & Nelson, D. R. (1988). *Phys. Rev. B*, **37**, 4458–4472.

Levine, D., Lubensky, T. C., Ostlund, S., Ramaswamy, S., Steindhardt, P. J. & Toner, J. (1985). *Phys. Rev. Lett.* **54**, 1520–1523.

Lubensky, T. C., Ramaswamy, S. & Toner, J. (1985). *Phys. Rev. B*, **32**, 7444–7452.

Nye, J. F. (1957). *Physical Properties of Crystals.* Oxford: Clarendon Press.

Socolar, J. E. S. (1989). *Phys. Rev. B*, **39**, 10519–10551.