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Analytical expressions of the elastic displacement fields induced by straight dislocations in decagonal, octagonal and dodecagonal quasicrystals

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Abstract. According to the generalized Eshelby *et al* (1953 *Acta Metall.* **1** 251) method of a straight dislocation line in quasicrystals (QCs), the analytical expressions for elastic displacement fields induced by dislocations in decagonal, octagonal and dodecagonal QCs have been derived when the dislocation lines are parallel to some symmetry axes.

1. Introduction

During the last few years, dislocations have been observed in quasicrystals (QCs) by transmission electron microscopy (TEM), and their Burgers vectors have been identified experimentally using diffraction contrast imaging [1–4] and convergent-beam electron diffraction [5, 6] techniques. In order to understand the effect of dislocations on the properties of QCs and to simulate the electron micrographs relevant to dislocations in QCs, the elasticity theory of dislocations, including the expressions for the elastic fields induced by these defects in QCs are a prerequisite. It is well known that the systematic theory of elasticity of defects in periodic crystals was established more than 20 years ago as summarized in [7, 8], but the problem for QCs is more difficult than in crystals.

Recently, the elastic constant matrices $[C]$, $[K]$ and $[R]$ for many types of QC were derived [9, 10] and a generalized elasticity theory of QCs was established [11]. Then an elastic model of dislocations in QCs based on the Green function method was suggested by Ding *et al* [12], and some analytical expressions for the displacement fields of straight dislocation lines were derived both in decagonal [12] and in dodecagonal [13] QCs.

On the other hand, in the case of crystals, besides the Green function method, there are other methods. An example is the method developed by Eshelby *et al* [14]. Recently Ding *et al* [15] have generalized the Eshelby *et al* method to the case of QCs and obtained expressions for the elastic fields of straight dislocation lines. The purpose of this paper is to apply the generalized Eshelby *et al* method to derive analytical expressions for the elastic displacement fields for some special straight dislocation lines in two-dimensional (2D) QCs. According to conventions of QC research [9, 10], hereafter a 2D QC refers not to a plane but to a three-dimensional (3D) body periodically stacked in a 2D quasiperiodic structure.

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2. Basic theoretical model

QCs possess two types of displacement field: one is the phonon field $\boldsymbol{u}(\boldsymbol{r})$ in the physical subspace, and the other is the phason field $\boldsymbol{w}(\boldsymbol{r})$ in the perpendicular subspace, where $\boldsymbol{r}$ is the position vector in the physical subspace. They satisfy the homogeneous partial differential equations (omitting the body force f_i and g_i) [11]:

$$\begin{aligned} C'_{ijkl}\partial_j\partial_l u_k + R'_{ijkl}\partial_j\partial_l w_k = 0 \\ R'_{klij}\partial_j\partial_l u_k + K'_{ijkl}\partial_j\partial_l w_k = 0 \end{aligned} \tag{1}$$

where the elastic constants C'_{ijkl} and K'_{ijkl} are associated with the phonon and phason fields, respectively, and R'_{ijkl} is associated with the possible coupling between the phonon and phason fields. They are referred to the conventional coordinate systems. The symbol $\partial_j \equiv \partial/\partial x_j$, and the subscripts i, j, k, l can be 1, 2 or 3. By choosing a dislocation orthogonal coordinate system (x_1, x_2, x_3) in the physical subspace with the x_3 axis parallel to the dislocation line and the corresponding coordinate system in the perpendicular subspace, and after transforming elastic constants to these systems, equation (1) has the following form:

$$\begin{aligned} C_{iJkL}\partial_J\partial_L u_k + R_{iJkL}\partial_J\partial_L w_k = 0 \\ R_{kLiJ}\partial_J\partial_L u_k + K_{iJkL}\partial_J\partial_L w_k = 0 \end{aligned} \tag{2}$$

where C_{iJkL}, K_{iJkL} and R_{iJkL} are all referred to the dislocation coordinate system. J and L take only the values 1 and 2.

Now we introduce the following symbols:

$$\mathcal{V}^{\beta}(\boldsymbol{r}) = \delta_k^{\beta} u_k(\boldsymbol{r}) + \delta_k^{\beta-3} w_k(\boldsymbol{r}) \tag{3}$$

$$B_{jl}^{\alpha\beta} = \delta_i^{\alpha}(\delta_k^{\beta} C_{ijkl} + \delta_k^{\beta-3} R_{ijkl}) + \delta_i^{\alpha-3}(\delta_k^{\beta} R_{klij} + \delta_k^{\beta-3} K_{ijkl}) \tag{4}$$

where

$$\delta_i^{\alpha} = \begin{cases} 1 & \alpha = i \\ 0 & \alpha \neq i \end{cases} \tag{5}$$

and the Greek letters α, β take the values 1, 2, 3, 4, 5 and 6.

By using these symbols, equation (2) can be rewritten as the standard form

$$B_{JL}^{\alpha\beta}\partial_J\partial_L V^{\beta}(\boldsymbol{r}) = 0. \tag{6}$$

According to Eshelby *et al* [14], equation (6) has solutions of the type

$$\mathcal{V}^{\beta}(\boldsymbol{r}) = A^{\beta} f(\eta) \tag{7}$$

where

$$\eta = x_1 + p x_2 \tag{8}$$

with p being a constant to be determined as follows.

If we substitute equation (7) into (6) and introduced a 6×6 matrix

$$a^{\alpha\beta} = B_{11}^{\alpha\beta} + (B_{12}^{\alpha\beta} + B_{21}^{\alpha\beta})p + B_{22}^{\alpha\beta} p^2 \tag{9}$$

then a set of linear algebraic equations for A^{β} can be obtained as follows:

$$a^{\alpha\beta} A^{\beta} = 0. \tag{10}$$

The parameter p in equation (8) is determined by the condition

$$\det|a^{\alpha\beta}| = 0. \tag{11}$$

Following the analogous procedure proposed by Eshelby *et al* [14], the displacements induced by an infinite straight dislocation line parallel to the positive x_3 axis can be expressed by the form

$$V^{\beta}(\boldsymbol{r}) = \mathrm{Re}\left[\sum_{n=1}^{6} \frac{1}{\pm 2\pi\mathrm{i}} A^{\beta}(n) D(n) \ln[\eta(n)]\right] \tag{12}$$

where Re means that only the real part is to be taken, the sign of $2\pi\mathrm{i}$ is taken to be the same as the sign of the imaginary part of $p(n)$, and the six complex constants $D(n)$ are determined by the following 12 equations

$$\mathrm{Re}\left[\sum_{n=1}^{6} A^{\beta}(n) D(n)\right] = b^{\beta} \tag{13}$$

$$\mathrm{Re}\left[\sum_{n=1}^{6} (B_{21}^{\alpha\beta} + B_{22}^{\alpha\beta} p(n)) A^{\beta}(n) D(n)\right] = 0 \tag{14}$$

where b^{β} are the components of the Burgers vector $\tilde{\boldsymbol{b}}$ of the dislocation.

3. Conditions for analytical solutions

A main crux in the generalized Eshelby *et al* method is to deal with solutions of a twelfth-order equation for p. As we know, unfortunately, only polynomials of fourth or lower order can be solved by general algebraic methods. Therefore, in order to obtain the elastic fields induced by straight dislocation line in QCs, we must in general employ some numerical calculations. However, it is still possible to find analytical expressions for the elastic fields in some special conditions. The key to the question is whether equation (10) can be separated into two independent and lower-dimensional sets of equations which can be solved by an algebraic method.

It is apparent that, if the elements

$$\begin{aligned} a^{13} &= a^{23} = a^{43} = a^{53} = a^{16} = a^{26} = a^{46} = a^{56} = a^{31} = a^{32} = a^{34} = a^{35} = a^{61} = a^{62} \\ &= a^{64} = a^{65} = 0 \end{aligned} \tag{15}$$

of the matrix $a^{\alpha\beta}$ are all equal to zero, then the set of equations (10) is separated into the following two independent sets: one set for A^1, A^2, A^4 and A^5 given by

$$\begin{aligned} &a^{11}A^1 + a^{12}A^2 + a^{14}A^4 + a^{15}A^5 = 0 \\ &[3pt]a^{21}A^1 + a^{22}A^2 + a^{24}A^4 + a^{25}A^5 = 0 \\ &[3pt]a^{41}A^1 + a^{42}A^2 + a^{44}A^4 + a^{45}A^5 = 0 \\ &[3pt]a^{51}A^1 + a^{52}A^2 + a^{54}A^4 + a^{55}A^5 = 0 \end{aligned} \tag{16}$$

and the other set for A^3 and A^6 given by

$$\begin{aligned} &a^{33}A^3 + a^{36}A^6 = 0 \\ &[3pt]a^{63}A^3 + a^{66}A^6 = 0. \end{aligned} \tag{17}$$

The conditions in equation (15) are true provided that the following elastic constants which refer to the dislocation coordinate system are all equal to zero:

$$C_{14} = C_{15} = C_{24} = C_{25} = C_{46} = C_{56} = 0 \tag{18}$$

$$\begin{aligned} K_{1131} &= K_{1132} = K_{2231} = K_{2232} = K_{3111} = K_{3122} = K_{3112} = K_{3121} = K_{1231} = K_{1232} \\ &= K_{3211} = K_{3222} = K_{3212} = K_{3221} = K_{2131} = K_{2132} = 0 \end{aligned} \tag{19}$$

$$\begin{aligned} R_{1131} &= R_{1132} = R_{2231} = R_{2232} = R_{3111} = R_{3122} = R_{3112} = R_{3121} = R_{1231} = R_{1232} \\ &= R_{3211} = R_{3222} = R_{3212} = R_{3221} = R_{2131} = R_{2132} = 0. \end{aligned} \tag{20}$$

When $I, J, K = 1$ or 2, a twofold rotation around the x_3 axis transforms C_{IJK3} into $-C_{IJK3}$ and hence we have $C_{IJK3} = 0$ if the x_3 axis is parallel to an even-fold symmetry axis. Each elastic constant in equations (18)–(20) contains one subscript 3 and hence will be equal to zero if the x_3 axis is parallel to an even-fold symmetry axis. Therefore, if a dislocation line in a 2D QC is parallel to an even-fold symmetry axis, then conditions (18)–(20) are fulfilled and equation (10) can be separated into two independent equations (16) and (17).

According to the dislocation condition (13), A^1, A^2, A^4 and A^5 are associated with the Burgers vector components $b_1^{\parallel}$, $b_2^{\parallel}$, $b_1^{\perp}$ and $b_2^{\perp}$, respectively, which are all perpendicular to the dislocation line, and A^3 and A^6 are associated with $b_3^{\parallel}$ and $b_3^{\perp}$ where the physical component $b_3^{\parallel}$ is parallel to the dislocation line. Hence, the conditions in equation (15) give rise to a separation of the solutions into two parts corresponding to the pure edge and pure screw dislocations.

Obviously, the solutions of the set of equations (17) can be obtained by the algebraic method because only a fourth-order equation in p is involved. It follows that analytical expressions of the elastic fields induced by a pure screw dislocation line parallel to an even-fold symmetry axis can be obtained.

However, to solve the set of equations (16), one will deal with solving an eighth-order equation in p. It appears that the conditions in equation (15) are not enough to give an analytical expression for pure edge dislocations. However, if the x_1 (or x_2) axis in the defect coordinate system is also an even-fold symmetry axis in addition to the x_3 axis, or equivalently if the x_2–x_3 plane (or if the x_1–x_3 plane) is a mirror plane, then the displacement vector $V^{\beta}(x_1, x_2)$ must be equal to $V^{\beta}(x_1, -x_2)$ and hence $\eta = x_1 + px_2$ and $\eta = x_1 - px_2$ must appear simultaneously. Thus the roots must occur in pairs $(p_1, -p_1)$, $(p_2, -p_2)$, $(p_4, -p_4)$ and $(p_5, -p_5)$. As a result, the determinant of the coefficient matrix of equation (16) must be of the form

$$(p^2 - p_1^2)(p^2 - p_2^2)(p^2 - p_4^2)(p^2 - p_5^2) = 0. \tag{21}$$

Hence, in this case, we also have to solve only a fourth-order algebraic equation in p^2.

4. Derivation of analytical expressions

In this section we shall apply the generalized Eshelby *et al* method to dislocation lines along even-fold (twofold, eightfold, tenfold or twelvefold) axes in 2D QCs to derive analytical expressions for their elastic displacement fields. The 2D QC considered here is a 3D body with a periodic axis and a 2D quasiperiodic plane.

4.1. Dislocation line lying in the quasiperiodic plane of octagonal two-dimensional quasicrystals

In the conventional QC coordinate system of octagonal 2D QCs, i.e. the x_3' axis parallel to the periodic direction and the x_1' axis parallel to one of the twofold axes in the quasiperiodic plane, the elastic constants of octagonal QCs with point groups $8/mmm$, $8mm$, 822 and $\bar{8}m2$ can be deduced from [9, 10] to be

$$
\begin{aligned}
&C'_{ijkl}(C_{KM}) : C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66} = \tfrac{1}{2}(C_{11} - C_{12}) \\
&K'_{ijkl} : K'_{1111} = K'_{2222} = K_1 \qquad K'_{1122} = K'_{2211} = K_2 \qquad K'_{1221} = K'_{2112} = K_3 \\
&\qquad\qquad K'_{1313} = K'_{2323} = K_4 \qquad K'_{2121} = K'_{1212} = K_1 + K_2 + K_3 \\
&R'_{ijkl} : R'_{1111} = R'_{1122} = -R'_{2211} = -R'_{2222} = R'_{1221} = R'_{2121} = -R'_{1212} = -R'_{2112} = R.
\end{aligned}
$$

Consider a straight dislocation line $\boldsymbol{t}$ parallel to the x'_1 axis which is a twofold axis. We choose a dislocation coordinate system (x_1, x_2, x_3) in which the x_3 axis is along the positive direction of $\boldsymbol{t}$ in the physical space, and the x_2 axis is along the periodic axis. This system can be obtained from the conventional QC system by the following subscript transformation: $1' \to 3$, $2' \to 1$, $3' \to 2$. In the present paper, we take the same relationship between the dislocation system $x_1^{\perp}$, $x_2^{\perp}$ and $x_3^{\perp}$ and the QC system $x_1^{\perp'}$, $x_2^{\perp'}$ and $x_3^{\perp'}$ in perpendicular subspace, i.e. in this case we have $x_1^{\perp'} \to x_3^{\perp'}$, $x_2^{\perp'} \to x_1^{\perp'}$ and $x_3^{\perp'} \to x_2^{\perp}$. Then the non-vanishing elastic constants in the dislocation coordinate system are as follows:

$$
\begin{aligned}
&C_{iJkL} : C_{1111} = C_{11} \qquad C_{2222} = C_{33} \qquad C_{1122} = C_{2211} = C_{13} \qquad C_{3131} = C_{66} \\
&\qquad\qquad C_{1212} = C_{2121} = C_{1221} = C_{2112} = C_{3232} = C_{44} \\
&K_{iJkL} : K_{1111} = K_1 \qquad K_{3131} = K_1 + K_2 + K_3 \qquad K_{1212} = K_{3232} = K_4 \\
&R_{iJkL} : R_{1111} = R_{3131} = -R.
\end{aligned}
$$

In this case, the x_1 and x_3 axes are all even-fold symmetrical. It is certain that analytical expressions can be found. Equation (10) consists of five equations and is separated into two independent sets of equations: one set for A^1, A^2 and A^4 given by

$$
\begin{aligned}
&(C_{11} + C_{44}p^2)A^1 + (C_{13} + C_{44})pA^2 - RA^4 = 0 \\
&(C_{13} + C_{44})pA^1 + (C_{44} + C_{33}p^2)A^2 = 0 \\
&-RA^1 + (K_1 + K_4p^2)A^4 = 0
\end{aligned}
\tag{22}
$$

with $p(n) = p(1)$, $p(2)$, $p(4)$, $p(7)$, $p(8)$ and $p(10)$, and the other set for A^3 and A^6 given by

$$
\begin{aligned}
&(C_{66} + C_{44}p^2)A^3 - RA^6 = 0 \\
&-RA^3 + [(K_1 + K_2 + K_3) + K_4p^2]A^6 = 0
\end{aligned}
\tag{23}
$$

with $p(n) = p(3)$, $p(6)$, $p(9)$ and $p(12)$.

Correspondingly, equation (11) also consists of two independent algebraic equations for p:

$$
\begin{aligned}
&C_{33}C_{44}K_4p^6 + [K_4(C_{11}C_{33} - C_{13}^2 - 2C_{13}C_{44}) + C_{33}C_{44}K_1]p^4 + [C_{11}C_{44}K_4 - C_{33}R^2 \\
&\qquad + K_1(C_{11}C_{33} - C_{13}^2 - 2C_{13}C_{44})]p^2 + C_{44}(C_{11}K_1 - R^2) = 0
\end{aligned}
\tag{24}
$$

and

$$
C_{44}K_4p^4 + [C_{66}K_4 + C_{44}(K_1 + K_2 + K_3)]p^2 + C_{66}(K_1 + K_2 + K_3) - R^2 = 0. \tag{25}
$$

Now we consider only the elastic displacement field of the screw component of the dislocation with $\tilde{b} = (0, 0, b_3^{\parallel}, 0, b_3^{\perp})$. Obviously, we have to solve only equations (23) and (25). Equation (25) has two pairs of complex conjugate roots. Pick out two roots $p(3)$ and $p(6)$ with a positive imaginary part:

$$
p(3) = \sqrt{\frac{s_1 + s_2}{2C_{44}K_4}}\,\mathrm{i} \qquad p(6) = \sqrt{\frac{s_1 - s_2}{2C_{44}K_4}}\,\mathrm{i} \tag{26}
$$

where

$$s_1 = C_{66}K_4 + C_{44}(K_1 + K_2 + K_3) \tag{27}$$

$$s_2^2 = [C_{66}K_4 - C_{44}(K_1 + K_2 + K_3)]^2 + 4C_{44}K_4R^2. \tag{28}$$

We arbitrarily put $A^3(3) = A^3(6) = 1$ and obtain from equation (23) the result

$$A^6(3) = \frac{2C_{44}R}{s_1 - s_2 - 2C_{66}K_4} \tag{29}$$

$$A^6(6) = \frac{2C_{44}R}{s_1 + s_2 - 2C_{66}K_4}. \tag{30}$$

Substituting equations (26), (29) and (30) into equations (13) and (14), and considering $n = 3$, 6 and $b^3 = b_3^{\parallel}$, $b^6 = b_3^{\perp}$, we have

$$D(3) = \frac{s_2 - s_1 + 2C_{66}K_4}{2s_2} b_3^{\parallel} - \frac{K_4R}{s_2} b_3^{\perp} \tag{31}$$

$$D(6) = \frac{s_2 + s_1 - 2C_{66}K_4}{2s_2} b_3^{\parallel} + \frac{K_4R}{s_2} b_3^{\perp}. \tag{32}$$

Finally, since all the quantities needed for equation (12) are now given explicitly in equations (26) and (29)–(32), one can find the displacement fields induced by a dislocation with $\tilde{\boldsymbol{b}} = (0, 0, b_3^{\parallel}, 0, b_3^{\perp})$ as follows:

$$\begin{aligned} V^3 = u_3(\boldsymbol{r}) = \frac{1}{4\pi s_2} \Bigg[&[(s_2 - s_1 + 2C_{66}K_4)b_3^{\parallel} - 2K_4Rb_3^{\perp}] \tan^{-1}\left(\sqrt{\frac{s_1 + s_2}{2C_{44}K_4}} \frac{x_2}{x_1}\right) \\ &+ [(s_2 + s_1 - 2C_{66}K_4)b_3^{\parallel} + 2K_4Rb_3^{\perp}] \tan^{-1}\left(\sqrt{\frac{s_1 - s_2}{2C_{44}K_4}} \frac{x_2}{x_1}\right)\Bigg] \end{aligned} \tag{33}$$

$$\begin{aligned} V^6 = w_3(\boldsymbol{r}) = \frac{C_{44}R}{2\pi s_2} \Bigg[&\left(-b_3^{\parallel} - \frac{2K_4R}{s_1 - s_2 - 2C_{66}K_4} b_3^{\perp}\right) \tan^{-1}\left(\sqrt{\frac{s_1 + s_1}{2C_{44}K_4}} \frac{x_2}{x_1}\right) \\ &+ \left(b_3^{\parallel} + \frac{2K_4R}{s_1 + s_2 - 2C_{66}K_4} b_3^{\perp}\right) \tan^{-1}\left(\sqrt{\frac{s_1 - s_2}{2C_{44}K_4}} \frac{x_2}{x_1}\right)\Bigg]. \end{aligned} \tag{34}$$

As a check, the formulae for the anisotropic case in a hexagonal crystal can be obtained by limiting procedures, e.g. putting $R = 0$ and $K_1, K_2, K_3, K_4 \to 0$.

Equation (24), corresponding to the edge component of the dislocation with $\tilde{\boldsymbol{b}} = (b_1^{\parallel}, b_2^{\parallel}, 0, b_1^{\perp}, 0)$, is third order in p^2 and can be solved algebraically, but the calculations are very cumbersome and are omitted here for brevity.

4.2. Dislocation line lying in the quasiperiodic plane of a decagonal two-dimensional quasicrystal

4.2.1. Dislocation line parallel to the A2P axis. The elastic constants of a decagonal QC with point groups $10/mmm$, $10mm$, 1022 and $\overline{10}m2$ are the same as those of the octagonal QC except K_3 in the octagonal QC should be replaced by $-K_2$. Therefore, all the corresponding formulae for the decagonal QC can be obtained by substituting $-K_2$ for K_3, and the expressions for the displacement fields induced by a screw dislocation line parallel to a twofold axis (A2P) in the decagonal QC are the same as equations (33) and (34), except for parameters s_1 and s_2 which should be changed to

$$s_1 = C_{66}K_4 + C_{44}K_1 \tag{35}$$

$$s_2^2 = (C_{66}K_4 - C_{44}K_1)^2 + 4C_{44}K_4R^2. \tag{36}$$

4.2.2. Dislocation line parallel to the A2D axis. As is known, there are two different types of twofold axis in the quasiperiodic plane of the decagonal QC, i.e. A2P and A2D axes. Now we consider a screw dislocation line parallel to the A2D axis and still choose a dislocation coordinate system in which the x_3 axis is along the dislocation line. The x_2 axis is along the periodic direction. This system can be obtained from the conventional QC system by the following subscript transformation: $1' \to 1$, $2' \to -3$, $3' \to 2$. After the transformations, we find that all the elastic constants in this coordinate system are the same as those in the coordinate system of section 4.2.1 except that R is replaced by $-R$. This means that there is no difference between the elastic properties of the A2P axis and the A2D axis. Therefore, if the dislocation line is parallel to an A2D axis, then the expressions are the same as equations (33) and (34) with the substitution of $-K_2$ for K_3 and $-R$ for R. This case was discussed in detail in [15] and we repeat it here for the completeness of the present paper.

4.3. Dislocations in dodecagonal quasicrystals

4.3.1. Dislocation line in the quasiperiodic plane. The elastic constants of the dodecagonal QC with point groups $12/mmm$, $12mm$, 1222 and $\overline{12}m2$ are the same as those of the octagonal QC with $R = 0$. Therefore, the formulae for the displacements induced by a screw dislocation lying in the quasiperiodic plane and along the A2P axis in dodecagonal QCs can be obtained directly from equations (33) and (34) by limiting procedures. When $R = 0$, equation (33) yields

$$V^3 = u_3(r) = \frac{b_3^{\parallel}}{2\pi} \tan^{-1}\left(\sqrt{\frac{C_{66}}{C_{44}}}\frac{x_2}{x_1}\right). \tag{37}$$

Care is required for equation (34), e.g. $s_2 = C_{66}K_4 - C_{44}(K_1 + K_2 + K_3) + 2C_{44}K_4R^2/[C_{66}K_4 - C_{44}(K_1 + K_2 + K_3)]$ as $R \to 0$, and

$$\lim_{R\to 0}\left(\frac{2K_4C_{44}R^2}{s_2(s_1 - s_2 - 2C_{66}K_4)}\right) = 0 \qquad \lim_{R\to 0}\left(\frac{2K_4C_{44}R^2}{s_2(s_1 + s_2 - 2C_{66}K_4)}\right) = 1.$$

Then equation (34) becomes

$$V^6 = w_3(r) = \frac{b_3^{\perp}}{2\pi} \tan^{-1}\left(\sqrt{\frac{K_1 + K_2 + K_3}{K_4}}\frac{x_2}{x_1}\right). \tag{38}$$

Now we shall discuss the pure edge dislocation. In this case, equation (22) reduces to two independent sets of equations due to $R = 0$: one set for A^1 and A^2 given by

$$\begin{aligned} &(C_{11} + C_{44}p^2)A^1 + (C_{13} + C_{44})pA^2 = 0 \\ &(C_{13} + C_{44})pA^1 + (C_{44} + C_{33}p^2)A^2 = 0 \end{aligned} \tag{39}$$

and the other for A^4 given by

$$(K_1 + K_4p^2)A^4 = 0. \tag{40}$$

Equation (39) is the same as that of the edge dislocation in crystals and the results with the Burgers vector components $(b_1, b_2, 0)$ have been given on pp 422–5 of [7]. Here we shall consider only the elastic displacement field induced by the Burgers vector $(b_1^{\perp}, 0)$, the accompanying component in the perpendicular subspace of the Burgers vector of the pure edge dislocation. Hence we have to solve only a second-order equation

$$K_1 + K_4p^2 = 0 \tag{41}$$

which has the solutions

$$p(4) = \sqrt{\frac{K_1}{K_4}}\mathrm{i} \qquad p(10) = -\sqrt{\frac{K_1}{K_4}}\mathrm{i}. \tag{42}$$

Let $A^4 \equiv 1$. Substituting equations (41) and (42) into equations (13) and (14), one can get

$$D(4) = b_1^{\perp}. \tag{43}$$

Finally the expression for the phason displacement of an edge dislocation with $\tilde{b} = (b_1^{\perp}, 0)$ can be given by

$$V^4 = w_1(r) = \frac{b_1^{\perp}}{2\pi} \tan^{-1}\left(\sqrt{\frac{K_1}{K_4}}\frac{x_2}{x_1}\right). \tag{44}$$

From the above, we have derived the expressions for the phason displacement field $\boldsymbol{w}$ corresponding to the components $(b_1^{\perp}, b_3^{\perp})$ as in equations (44) and (38).

4.3.2. Dislocation line parallel to the periodic direction. Now we consider a straight dislocation line, parallel to the periodic direction (x_3 axis) of a dodecagonal QC, with an arbitrary Burgers vector $\tilde{\boldsymbol{b}} = (b_1^{\parallel}, b_2^{\parallel}, 0, b_1^{\perp}, b_2^{\perp})$. In this case, equation (10) can be reduced to three independent sets of equations: one set for A^1 and A^2, the edge components in the physical subspace, given by

$$\begin{aligned}(C_{11} + C_{66}p^2)A^1 + (C_{12} + C_{66})pA^2 = 0\\ (C_{12} + C_{66})pA^1 + (C_{66} + C_{11}p^2)A^2 = 0\end{aligned} \tag{45a}$$

the second set for A^3, the screw component in the physical subspace, given by

$$(C_{44} + C_{44}p^2)A^3 = 0 \tag{45b}$$

and the third set for A^4 and A^5, the accompanying edge components in the perpendicular subspace, given by

$$\begin{aligned}(K_1 + \Sigma p^2)A^4 + (K_2 + K_3)pA^5 = 0\\ (K_2 + K_3)pA^4 + (\Sigma + K_1p^2)A^5 = 0\end{aligned} \tag{46}$$

where

$$\Sigma = K_1 + K_2 + K_3. \tag{47}$$

It can be seen from equation (45) that the expressions for the phonon displacement field $\boldsymbol{u}$ of the dislocation with the Burgers vector $\boldsymbol{b} = (b_1^{\parallel}, b_2^{\parallel}, b_3^{\parallel})$ will be the same as those of the dislocation in crystals. The results can be obtained from the anisotropic case by limiting procedures:

$$\begin{aligned}
u_1 &= \frac{b_2^{\parallel}}{2\pi}\left[\tan^{-1}\left(\frac{x_2}{x_1}\right) + \frac{C_{11} - C_{66}}{C_{11}}\frac{x_1x_2}{r^2}\right] + \frac{b_2^{\parallel}}{2\pi}\left[\frac{C_{66}}{C_{11}}\ln\left(\frac{r}{r_0}\right) - \frac{C_{11} - C_{66}}{C_{11}}\frac{x_1^2}{r^2}\right]\\
u_2 &= -\frac{b_1^{\parallel}}{2\pi}\left[\frac{C_{66}}{C_{11}}\left(\frac{r}{r_0}\right) - \frac{C_{11} - C_{66}}{C_{11}}\frac{x_2^2}{r^2}\right] + \frac{b_2^{\parallel}}{2\pi}\left[\tan^{-1}\left(\frac{x_2}{x_2}\right) - \frac{C_{11} - C_{66}}{C_{11}}\frac{x_1x_2}{r^2}\right]\\
u_3 &= \frac{b_3^{\parallel}}{2\pi}\tan^{-1}\left(\frac{x_2}{x_1}\right).
\end{aligned} \tag{48}$$

Here r_0 is the radius of the dislocation core.

Next we shall solve equation (46) and give the expression for the phason displacement field $\boldsymbol{w}$ corresponding to the perpendicular components $(b_1^{\perp}, b_2^{\perp})$ of the Burgers vector. Therefore, we have to solve only a fourth-order equation in p:

$$K_1\Sigma p^4 + [K_1^2 + \Sigma^2 - (K_2 + K_3)^2]p^2 + K_1\Sigma = 0. \tag{49}$$

The roots are of the form

$$\begin{aligned} &p(4) = \lambda \exp(\mathrm{i}\phi) \qquad p(10) = \lambda \exp(-\mathrm{i}\phi) \\ &p(5) = -\lambda \exp(\mathrm{i}\phi) \qquad p(11) = -\lambda \exp(-\mathrm{i}\phi). \end{aligned} \tag{50}$$

where λ and ϕ are given by

$$\begin{aligned} &\lambda = 1 \\ &\phi = \frac{1}{2}\cos^{-1}\left[\frac{(K_2+K_3)^2 - K_1^2 - \Sigma^2}{2K_1\Sigma}\right] = \frac{\pi}{2}. \end{aligned} \tag{51}$$

We arbitrarily put $A^4 = 1$ and obtain from equation (46) the result

$$A^5(4) = -A^5(5) = -\frac{K\exp(-\mathrm{i}\phi) + \Sigma\exp(\mathrm{i}\phi)}{K_2 + K_3}. \tag{52}$$

For convenience, we first consider $\boldsymbol{b} = (b_1^{\perp}, 0)$. Inserting equations (50) and (52) into equations (13) and (14) and putting $b^4 = b_1^{\perp}$, $b^5 = 0$, then we have

$$D(4) = -D(5) = \frac{b_1^{\perp}}{2}\left(1 - i\frac{K_2^2 + \Sigma^2 - K_1^2 - K_3^2}{2K_1\Sigma\sin(2\phi)}\right). \tag{53}$$

Finally, the phason displacement field induced by $(b_1^{\perp}, 0)$ can be obtained as follows:

$$\begin{aligned} V^4 = w_1 &= \frac{b_1^{\perp}}{4\pi}\left[\tan^{-1}\left(\frac{2x_1x_2\sin\phi}{x_1^2 - x_2^2}\right) - \frac{K_2^2 + \Sigma^2 - K_1^2 - K_3^2}{2K_1\Sigma\sin(2\phi)}\ln\left(\frac{q}{t}\right)\right] \\ V^5 = w_2 &= \frac{b_1^{\perp}}{4\pi(K_2+K_3)}\left\{\left[(K_1+\Sigma)\cos\phi - \frac{(K_1-\Sigma)(K_2^2+\Sigma^2-K_1^2-K_3^2)}{4K_1\Sigma\cos\phi}\right]\tan^{-1}\right. \\ &\quad \times\left(\frac{x_2^2\sin(2\phi)}{x_1^2 - x_2^2\cos(2\phi)}\right) \\ &\quad \left. + \left[(K_1-\Sigma)\sin\phi + \frac{(K_1+\Sigma)(K_2^2+\Sigma^2-K_2^2-K_3^2)}{4K_1\Sigma\sin\phi}\right]\ln(qt)\right\} \end{aligned} \tag{54}$$

where

$$\begin{aligned} q^2 &= x_1^2 + x_2^2 + 2x_1x_2\cos\phi \\ t^2 &= x_1^2 + x_2^2 - 2x_1x_2\cos\phi. \end{aligned} \tag{55}$$

The results for the Burgers vector components $(0, b_2^{\perp})$ can be obtained from the results above by rotation of our coordinate system by $\pi/2$ in the physical space and by $5\pi/2$ in the perpendicular space [13]. Combining these results, and using the limiting procedures

$$\phi \to \frac{\pi}{2}$$

and

$$\lim_{\phi\to\pi/2}\left(\frac{\tan^{-1}\{[x_2^2\sin(2\phi)]/[x_1^2 - x_2^2\cos(2\phi)]\}}{\cos\phi}\right) = \frac{2x_2^2}{x_1^2 + x_2^2}$$

$$\lim_{\phi\to\pi/2}\left(\frac{1}{\sin(2\phi)}\right)\ln\left(\frac{q}{t}\right) = \frac{x_1x_2}{x_1^2 + x_2^2}$$

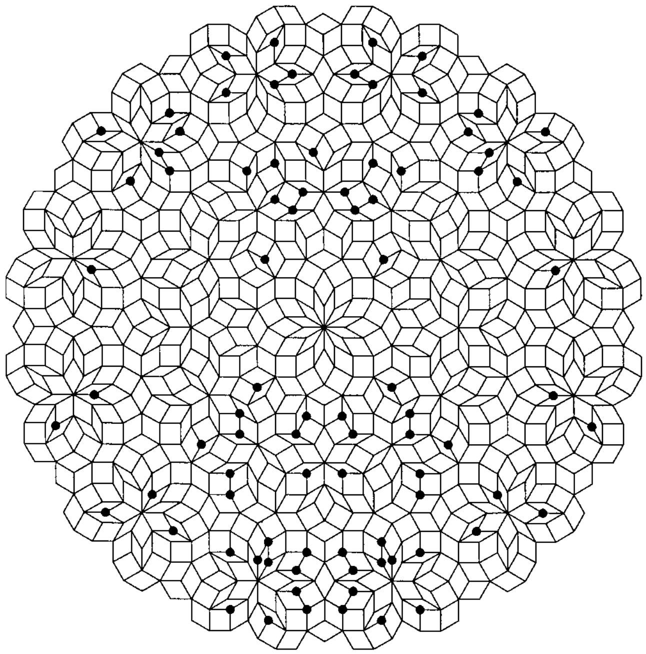

Figure 1. Section–projection diagram of a perfect dodecagonal QC perpendicular to the twelvefold axis.

one finds that the phason displacement fields of the dislocation with the Burgers vector components $(b_1^\perp, b_2^\perp)$ are

$$\begin{aligned} w_1 = {} & \frac{b_1^\perp}{2\pi}\left[\tan^{-1}\left(\frac{x_2}{x_1}\right) - \frac{(K_1+K_2)(K_2+K_3)}{2K_1(K_1+K_2+K_3)}\frac{x_1x_2}{r^2}\right] \\ & -\frac{b_2^\perp}{4\pi}\left[\frac{K_2(K_1+K_2+K_3)-K_1K_3}{K_1(K_1+K_2+K_3)}\ln\left(\frac{r}{r_0}\right) + \frac{(K_1+K_2)(K_2+K_3)}{K_1(K_1+K_2+K_3)}\frac{x_1^2}{r^2}\right] \\ w_2 = {} & \frac{b_1^\perp}{4\pi}\left[\frac{K_2(K_1+K_2+K_3)-K_1K_3}{K_1(K_1+K_2+K_3)}\ln\left(\frac{r}{r_0}\right) + \frac{(K_1+K_2)(K_2+K_3)}{K_1(K_1+K_2+K_3)}\frac{x_2^2}{r^2}\right] \\ & +\frac{b_2^\perp}{2\pi}\left[\tan^{-1}\left(\frac{x_2}{x_1}\right) + \frac{(K_1+K_2)(K_2+K_3)}{2K_1(K_1+K_2+K_3)}\frac{x_1x_2}{r^2}\right]. \end{aligned} \tag{56}$$

Thus, we have obtained the general expression for the elastic displacement fields of the dislocation with the Burgers vector $\tilde{\boldsymbol{b}} = (b_1^\parallel, b_2^\parallel, b_3^\parallel, b_1^\perp, b_2^\perp)$ as equations (48) and (56) when the dislocation line is along the periodic direction.

4.4. Screw dislocations parallel to even-fold periodic axes of two-dimensional quasicrystals

When a dislocation line is parallel to an even-fold periodic axis, e.g. eightfold, tenfold or twelvefold axis, of a 2D QC, then a^{36}, a^{63} and a^{66} in equation (17) all vanish and equation (17) is reduced to

$$(C_{44} + C_{44}p^2)A^3 = 0. \tag{57}$$

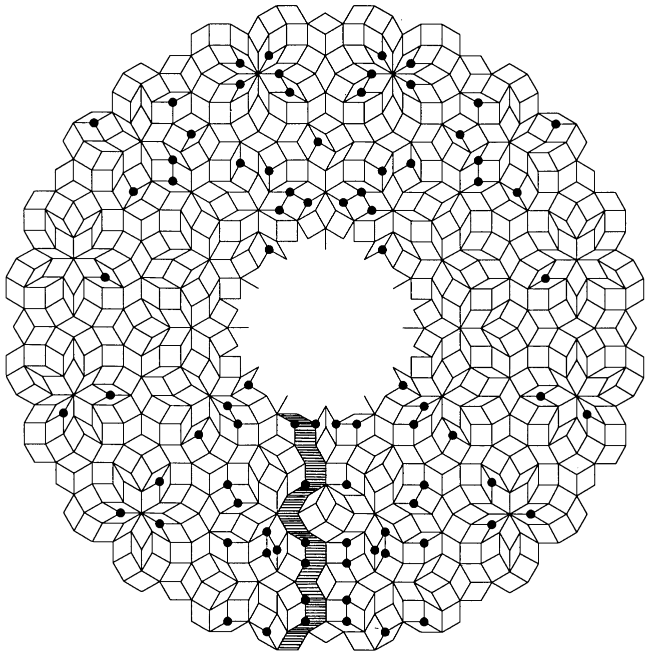

Figure 2. As for figure 1 but containing a dislocation, lying in the middle of the diagram and perpendicular to the diagram, with a fictitious Burgers vector [00010], showing the effect of the phason displacement. The lattice points indicated as full circles jump from the corresponding full circles indicated in figure 1.

By comparing it with equations (40) and (45*b*) one can find the expression for the phonon displacement for the screw dislocation with $\tilde{\boldsymbol{b}} = (0, 0, b_3^{\parallel}, 0, 0)$ as follows:

$$V^3(r) = u_3(r) = \frac{b_3^{\parallel}}{2\pi} \tan^{-1}\left(\frac{x_2}{x_1}\right) \tag{58}$$

which is exactly the displacement induced by a screw dislocation in an isotropic medium.

5. Section–projection diagrams of dodecagonal quasicrystal containing a dislocation line parallel to the periodic direction

In order to show the difference between the displacement fields in QCs discussed in the present paper and those in ordinary crystals, and also as an application of the expressions deduced above, we provide here section–projection diagrams of the dodecagonal QC containing a dislocation line parallel to the periodic x_3 direction with a Burgers vector $\tilde{\boldsymbol{b}} = [10010]$, i.e. $b_1^{\parallel} = 1$, $b_2^{\parallel} = 0$, $b_3^{\parallel} = 0$, $b_1^{\perp} = 1$ and $b_2^{\perp} = 0$ by using equations (48) and (56). The section–projection diagrams were proposed by Katz and Duneau [16] and applied by Wang and Wang [17] to describe the lattice model of a small dislocation loop in icosahedral quasicrystal.

Figures 1–3 are section–projection diagrams perpendicular to the twelvefold x_3 axis. In the calculation the following elastic constants were taken: $C_{66}/C_{11} = K_2/K_1 = K_3/K_1 = 0.3$. Figure 1 shows a perfect dodecagonal QC which appears as perfect twelvefold generalized Penrose tilting consisting of 30°, 60° and 90° rhombi. Figure 2 shows the diagram when

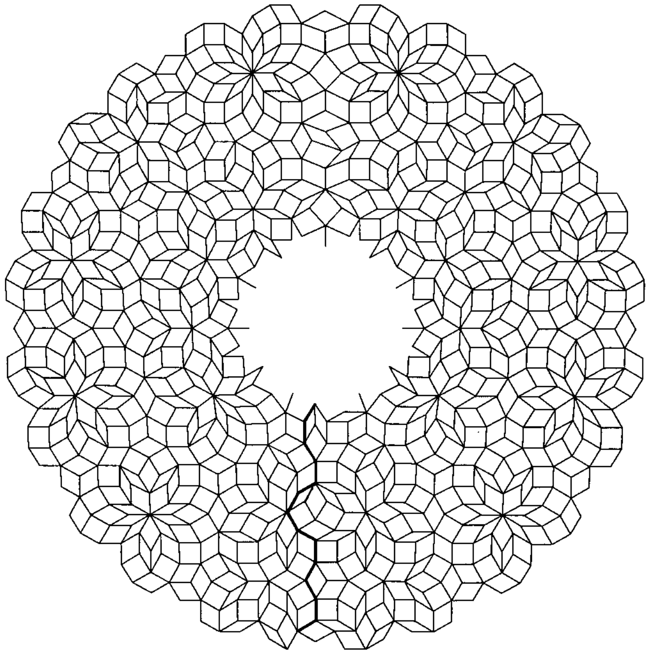

Figure 3. As for figure 2 but with a Burgers vector [10010]. The bold line shows the glued lips of the path removed in figure 2.

only phason strain is introduced, and figure 3 the diagram when both phason and phonon strains are introduced. Dislocation cores are removed in both figures 2 and 3. It must be emphasized that phason and phonon strains must be introduced simultaneously when the Burgers vector $\boldsymbol{b}^{\parallel}$ is along the quasiperiodic direction. We suppose that there is no phonon displacement field in figure 2 in order to show the effect of the phason displacement field. Of course this is not the real situation. By comparing figures 1 and 2 we can find that the phason displacements cause rearrangements of some quasilattice points that are indicated as full circles, i.e. the quasilattice points indicated as full circles in figure 1 jump to the corresponding full circles in figure 2. We can also find that there are several ways of jumping. Figure 4 summarizes 17 types of jumping where tiling diagrams of the perfect QC are drawn with solid lines and those generated by rearrangements caused by phason strain are drawn with broken lines. Figures 4(a), 4(b) and 4(c) show two, five and ten ways, respectively, by which only one, two and three points have jumped. All these rearrangements of lattice points are characteristic of QCs and do not happen in ordinary crystals. Moreover, we have shown a shaded path in figure 2. This path is removed and then the lips are glued together when the phonon strain is introduced as indicated by a bold line in figure 3. Figure 3 also shows that the phonon displacements cause distortion of the quasilattice in the dodecagonal QC.

6. Discussion

In this paper, after having summarized the generalized Eshelby *et al* method, we have discussed the conditions for obtaining analytical solutions and derived analytical expressions for the elastic displacement fields of some special dislocation lines in 2D QCs. By using

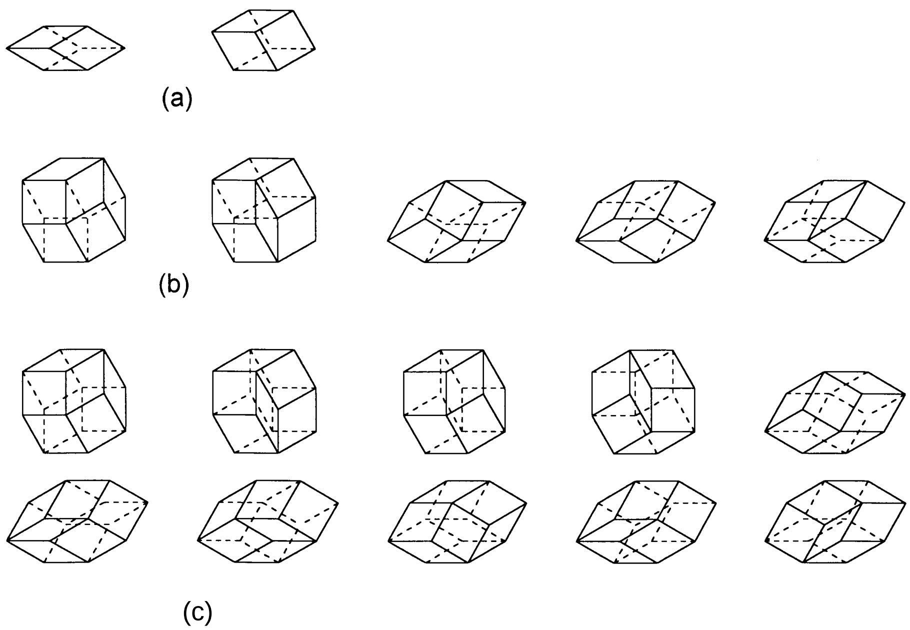

Figure 4. Tiling diagrams showing the ways of jumping caused by phason strain. (a) Tiling diagrams showing that only one point has jumped. (b) Tiling diagrams showing that two points have jumped simultaneously. (c) Tiling diagrams showing that three points have jumped simultaneously.

the Green function and eigenstrain methods, Yang *et al* [13] have calculated the elastic displacement fields of dislocation lines either parallel to the periodic direction or lying in the basal plane of a dodecagonal QC. Their results are in agreement with the expressions in the present paper. This agreement further confirms the correctness of both the Green function method and the generalized Eshelby *et al* method developed by us. In addition to the dislocation lines in dodecagonal QC, we have also derived the analytical expressions of the displacement fields of dislocation lines lying in the basal plane of octagonal and decagonal QCs for the first time.

According to our experience the generalized Eshelby *et al* method is sometimes complementary to the generalized Green function method for reducing analytical expressions of the displacement fields induced by straight dislocations in QCs. For example, Ding *et al* [12] succeeded in deducing analytical expressions for dislocation lines parallel to the periodic direction (A10 axis) of a decagonal QC by using the generalized Green function method but we have not succeeded by using the generalized Eshelby *et al* method. On the contrary, analytical expressions for dislocation lines lying in the quasiperiodic planes of octagonal and decagonal QCs are deduced by using a generalized Eshelby *et al* method in the present paper but have not been obtained by using the generalized Green functions method.

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References

[1] Wang Z G, Wang R and Deng W F 1991 *Phys. Rev. Lett.* **66** 2124
[2] Wang Z G, Wang R and Feng J L 1994 *Phil. Mag.* A **70** 577
[3] Feng J L and Wang R 1994 *J. Phys.: Condens. Matter* **6** 6437
[4] Wang R, Yang X, Zou W, Wang Z, Gui J and Jiang J 1994 *J. Phys.: Condens. Matter* **6** 9009
[5] Wang R and Dai M X 1993 *Phys. Rev.* B **47** 15 326
[6] Feng J L and Wang R 1994 *Phil. Mag.* A **69** 981
[7] Hirth J P and Lothe J 1968 *Theory of Dislocations* (New York: McGraw-Hill)
[8] Bacon D J, Barnett D M and Scattergood R O 1978 *Prog. Mater. Sci.* **23** 51
[9] Yang W G, Wang R, Ding D H and Hu C Z 1995 *J. Phys.: Condens. Matter* **7** 7099
[10] Hu C Z, Wang R, Yang W G and Ding D H 1996 *Acta Crystallogr.* A **52** 251
[11] Ding D H, Yang W G, Hu C Z and Wang R 1993 *Phys. Rev.* B **48** 7003
[12] Ding D H, Wang R, Yang W G and Hu C Z 1995 *J. Phys.: Condens. Matter* **7** 5423
[13] Yang W G, Lei J L, Ding D H, Wang R and Hu C Z 1995 *Phys. Lett.* **200A** 177
[14] Eshelby J D, Read W T and Shockley W 1953 *Acta Metall.* **1** 251
[15] Ding D H, Qin Y L, Wang R, Yang W G and Hu C Z 1995 *Acta Phys. Sin.* **4** 816
[16] Katz A and Dunneau M 1986 *J. Physique* **47** 181
[17] Wang Z G and Wang R 1993 *J. Phys.: Condens. Matter* **5** 2935