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# Elastic field for a straight dislocation in an icosahedral quasicrystal

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## Abstract

A straight dislocation in a three-dimensional icosahedral quasicrystal is studied. A solution considering phonon–phason coupling is observed; the phonon–phonon, phason–phason and phonon–phason interactions are revealed, in which a comparison between the present solution and other approximate solutions including the classic solution for crystals is given, and shows that the coupling effect is significant.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Since the discovery of the quasicrystal, the experimental and theoretical studies on the new structure of solids have made a great achievement. Almost 200 individual quasicrystals in different alloy systems have been produced so far. Many among them are stable thermodynamically, so the quasicrystal becomes a new material. The mechanical behaviour including elasticity and defects of the material is an important field of study, in which the theory and experimental observation of defects such as dislocations were reported [1–6]. According to the continuum theory of dislocations in the general scheme of quasicrystal elasticity theory [7], the explicit expressions for the elastic field, in particular for the displacement field, induced by a dislocation have been obtained in several quasicrystals [8–13]. The first work in this area may be that of De and Pelcovits [14], who analysed a dislocation in a planar pentagonal quasicrystal and gave the analytical expressions. Some analysis methods such as the Green function method [8], the Eshelby method [11] and the displacement function method [12] have been developed to derive analytical expressions for dislocation-induced elastic field in various quasicrystal systems. Furthermore, Fan *et al* [15] developed the theory on interaction between a dislocation group (also called a dislocation pile-up) and a crack; this creates the study on nonlinear fracture theory of quasicrystalline materials.

Up to now among 200 quasicrystals there are 96 kinds of icosahedral quasicrystals and 65 kinds of decagonal ones. This shows that the icosahedral quasicrystals play a central role in

these materials. The icosahedral quasicrystal is a three-dimensional one, with a huge number of field variables and field equations involving elasticity. Since the discovery there is no exact solution for the dislocation. Yang *et al* [16] developed the Green function method to study the solution of dislocation in the icosahedral quasicrystal, but only an approximate solution was obtained, in which the authors assumed that the coupling elastic constant  $R = 0$ , i.e. the phonon–phason is decoupled. The approximation leads to the result, that is, the phonon field and the phason field are independent from each other in the solution. Furthermore, the phonon component  $u_3$  is independent from  $u_1, u_2$  in their solution. But it is well known that the coupling effect between phonon and phason is very important. According to group theory, the most useful mathematical tool describing symmetry, among all quasicrystal systems observed to date, excepting a unique exception—the two-dimensional 12-fold symmetry quasicrystal, phonon and phason degrees of freedom are coupled. So the coupling effect is significant for studying the physical properties including mechanical properties for all quasicrystals (apart from the two-dimensional 12-fold symmetry quasicrystal) including icosahedral quasicrystals.

In order to illustrate this, we can look for the results of an uncoupled solution given by Yang *et al* [16]. This is the first solution of dislocation in icosahedral quasicrystals, and presents the meaning in the development of theory of dislocation of quasicrystals. The phonon field of the solution of Yang *et al* is quoted as equation (17) of our present paper; readers can find that the solution is a pure classic dislocation solution, which is independent from the phasons. The phason field given by Yang *et al* [16] is independent from the phonon field too. The nature of icosahedral quasicrystals has not been revealed in their solution. To further develop the theory of dislocation of quasicrystals, study exploring the realistic phonon–phonon, phason–phason and phonon–phason interactions is necessary.

This paper considers a straight dislocation in an icosahedral quasicrystal, where the dislocation line is parallel to the  $x_3$ -direction. A general solution is suggested by introducing a displacement function for a three-dimensional icosahedral quasicrystal given by Fan and Guo [17]. The analytical expressions for the displacement field induced by a dislocation are obtained based on the displacement function and Fourier analysis as follows.

## 2. General solution of the governing equations for plane elasticity of icosahedral quasicrystals

According to the description of a  $n$ -dimensional quasicrystal as a quasi-periodic structure which is periodic in  $(3 + n)$ -dimensional space ( $1 \leq n \leq 3$ ), the  $(3 + n)$ -dimensional space can be divided into the direct sum of two orthogonal subspaces, one being three-dimensional physical or parallel space,  $E_{\parallel}$ , and the other being  $n$ -dimensional perpendicular or complementary space,  $E_{\perp}$ . Therefore, for each quasicrystal, there are two orthogonal coordinate systems, one in  $E_{\parallel}$  and the other in  $E_{\perp}$ . In addition to the usual phonon displacements  $u_i$  and phonon strains  $\varepsilon_{ij}$  describing the local shift of atoms in  $E_{\parallel}$ , one must introduce the phason displacements  $w_i$  and phason strains  $w_{ij}$  to describe the local rearrangements of atoms in  $E_{\perp}$ . In this framework, the generalized Hooke law stands for [7]

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl} \quad H_{ij} = R_{kl ij}\varepsilon_{kl} + K_{ijkl}w_{kl} \quad (1)$$

with

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad w_{ij} = \frac{\partial w_i}{\partial x_j} \quad (2)$$

where  $\sigma_{ij}$  and  $H_{ij}$  are stresses in  $E_{\parallel}$  and  $E_{\perp}$  respectively,  $C_{ijkl}$  and  $K_{ijkl}$  elastic constants in phonon and the phason field respectively, and  $R_{ijkl}$  the phonon–phason coupling elastic

constants. If the coordinate system can be chosen with  $x_3$ -axis pointing towards a vertex of an icosahedral quasicrystal, we have

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (3)$$

and  $[K]$  and  $[R]$

$$[K] = \begin{bmatrix} K_1 & 0 & 0 & 0 & K_2 & 0 & 0 & K_2 & 0 \\ 0 & K_1 & 0 & 0 & -K_2 & 0 & 0 & K_2 & 0 \\ 0 & 0 & K_2 + K_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_1 - K_2 & 0 & K_2 & 0 & 0 & -K_2 \\ K_2 & -K_2 & 0 & 0 & K_1 - K_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_2 & 0 & K_1 & -K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -K_2 & K_1 - K_2 & 0 & -K_2 \\ K_2 & K_2 & 0 & 0 & 0 & 0 & 0 & K_1 - K_2 & 0 \\ 0 & 0 & 0 & -K_2 & 0 & 0 & -K_2 & 0 & K_1 \end{bmatrix} \quad (4)$$

$$[R] = R \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & -1 \\ 1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & -1 \\ 1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 \end{bmatrix}$$

where  $\lambda$  and  $\mu$  are the Lamé constants.

Now consider a straight dislocation along the  $x_3$ -axis; the field variables are independent from coordinate  $x_3$ , so the problem is reduced to a two-dimensional one. Fan and Guo [17] developed a displacement potential function method. In this paper we use the results but add some description, that is, for a plane elasticity problem in the  $x_1x_2$  plane of an icosahedral quasicrystal the phonon and phason displacement can be expressed in terms of  $G(x, y)$ , the displacement potential function, as follows ( $x_1 = x, x_2 = y$ ):

$$u_1 = R \frac{\partial^2}{\partial x \partial y} \nabla^2 \nabla^2 [\alpha \Pi_1 + \beta \Pi_2] G - Rc_0 \frac{\partial^2}{\partial x \partial y} \Lambda \left[ (3\mu - \lambda) \frac{\partial^4}{\partial x^4} + 10(\lambda + \mu) \alpha \frac{\partial^4}{\partial x^2 \partial y^2} - (5\lambda + 9\mu) \frac{\partial^4}{\partial y^4} \right] G$$

$$u_2 = R \nabla^2 \nabla^2 \left[ \alpha \frac{\partial^2}{\partial y^2} \Pi_1 - \beta \frac{\partial^2}{\partial x^2} \Pi_2 \right] G - Rc_0 \Lambda^2 \left[ (\lambda + 2\mu) \frac{\partial^6}{\partial x^6} - 5(2\lambda + 3\mu) \alpha \frac{\partial^6}{\partial x^4 \partial y^2} + 5\lambda \frac{\partial^6}{\partial x^2 \partial y^4} + \mu \frac{\partial^6}{\partial y^6} \right] G \quad (5)$$

$$u_3 = -c_1 \frac{\partial^2}{\partial x \partial y} \left[ (\lambda + \mu) R^2 \Lambda^2 \Pi_1 \Pi_2 - (\lambda + 2\mu) \alpha \frac{\partial^2}{\partial y^2} \Pi_1^2 - \mu \beta \frac{\partial^2}{\partial x^2} \Pi_2^2 \right] G$$

$$w_1 = \frac{\partial^2}{\partial x \partial y} \nabla^2 [ -(\lambda + \mu) R^2 \Pi_1 \Pi_2 + 2c_0 \mu (\lambda + 2\mu) \Lambda^2 \nabla^2 ] G$$

$$w_2 = \nabla^2 \left[ \mu (\lambda + 2\mu) c_0 \Lambda^2 \Lambda^2 \nabla^2 - (\lambda + 2\mu) \alpha \frac{\partial^2}{\partial y^2} \Pi_1^2 - \mu \beta \frac{\partial^2}{\partial x^2} \Pi_2^2 \right] G$$

$$w_3 = -c_2 \frac{\partial^2}{\partial x \partial y} \left[ (\lambda + \mu) R^2 \Lambda^2 \Pi_1 \Pi_2 - (\lambda + 2\mu) \alpha \frac{\partial^2}{\partial y^2} \Pi_1^2 - \mu \beta \frac{\partial^2}{\partial x^2} \Pi_2^2 \right] G;$$

then the field equations mentioned above will be satisfied if

$$\nabla^2 \nabla^2 \nabla^2 \nabla^2 \nabla^2 G(x, y) + \nabla^2 LG(x, y) = 0 \quad (6)$$

where

$$\begin{aligned}\alpha &= \mu K_1 - R^2 & \beta &= (\lambda + 2\mu)K_1 - R^2 \\ c_0 &= \frac{\mu K_2^2 + (K_1 - 3K_2)R^2}{\mu(K_1 - K_2) - R^2} & c_1 &= \frac{(K_1 - K_2)R}{\mu(K_1 - K_2) - R^2} & c_2 &= \frac{(K_2\mu - R^2)}{\mu(K_1 - K_2) - R^2} \\ \Pi_1 &= 3\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}, & \Pi_2 &= 3\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2}, \\ \nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, & \Lambda^2 &= \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\end{aligned}\quad (7)$$

$$\begin{aligned}L &= \frac{c_0 R}{\mu\beta} \left[ -\frac{\partial^{10}}{\partial x^{10}} + 5 \left( 4 - 5 \frac{\lambda + 2\mu\alpha}{\mu\beta} \right) \frac{\partial^{10}}{\partial x^8 \partial y^2} - 10 \left( 11 - 10 \frac{\lambda + 2\mu\alpha}{\mu\beta} \right) \frac{\partial^{10}}{\partial x^6 \partial y^4} \right. \\ &\quad + 10 \left( 10 - 11 \frac{\lambda + 2\mu\alpha}{\mu\beta} \right) \frac{\partial^{10}}{\partial x^4 \partial y^6} - 5 \left( 5 - 4 \frac{\lambda + 2\mu\alpha}{\mu\beta} \right) \frac{\partial^{10}}{\partial x^2 \partial y^8} \\ &\quad \left. - \frac{\lambda + 2\mu\alpha}{\mu\beta} \frac{\partial^{10}}{\partial y^{10}} \right].\end{aligned}\quad (8)$$

If  $R^2/(\mu K_1) \ll 1$  (this is natural, because the coupling elastic constant is less than those of phonon and phason), equation (7),

$$\beta/\alpha \rightarrow 1. \quad (9)$$

Substituting (9) into (8) then into (6), we find that

$$\nabla^2 \nabla^2 \nabla^2 \nabla^2 \nabla^2 G(x, y) = 0. \quad (10)$$

The problem for determining displacement and stress fields induced by a dislocation is reduced to solving the boundary value problem of equation (10) under appropriate boundary conditions.

### 3. Solution to a dislocation in an icosahedral quasicrystal

Utilizing the formulae of a general solution suggested above and the Fourier transform technique, the analytical solution for a dislocation along the  $x_3$ -axis in an icosahedral quasicrystal can be obtained. Considering a dislocation with the core at the origin, the Burgers vector is denoted as  $b = b^{\parallel} \oplus b^{\perp} = (b_1^{\parallel}, b_2^{\parallel}, b_3^{\parallel}, b_1^{\perp}, b_2^{\perp}, b_3^{\perp})$ , where

$$\oint du_j = b_j^{\parallel} \quad \oint dw_j = b_j^{\perp} \quad (11)$$

in which the integrals in (11) should be taken along the Burgers circuit surrounding the dislocation core in  $E_{\parallel}$  [18]. Here we calculate only the elastic field for a typical problem, corresponding to  $b_1^{\parallel} \neq 0, b_1^{\perp} \neq 0, b_2^{\parallel} = b_3^{\parallel} = 0, b_2^{\perp} = b_3^{\perp} = 0$ .

For simplicity we can solve a half-plane problem, by considering symmetry and anti-symmetry of relevant field variables, so there are the following boundary conditions including the dislocation condition:

$$\sigma_{22}(x, 0) = \sigma_{32}(x, 0) \quad (12a)$$

$$= 0 \quad (12b)$$

$$H_{22}(x, 0) = H_{32}(x, 0) \quad (12c)$$

$$= 0 \quad (12d)$$

$$\oint du_1 = b_1^{\parallel} \quad (12e)$$

$$\oint dw_1 = b_1^\perp. \tag{12f}$$

In addition there are boundary conditions at infinity:

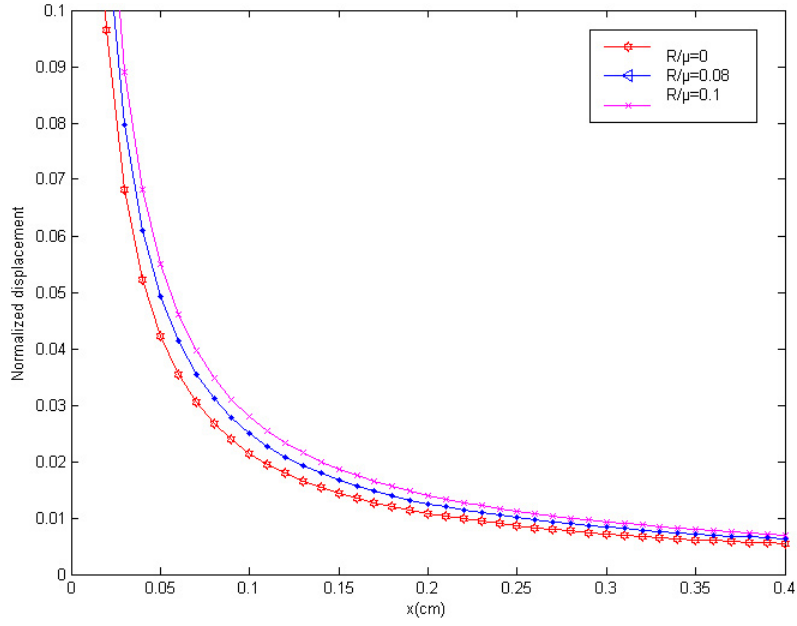
$$\sigma_{ij}(x, y) \rightarrow 0 \quad H_{ij}(x, y) \rightarrow 0 \quad \sqrt{x^2 + y^2} \rightarrow \infty. \tag{13}$$

Performing the Fourier transform to equation (10) and solving the corresponding ordinary differential at the transformed domain then taking the Fourier inversion, we obtain the solution as follows:

$$\begin{aligned} u_1 &= \frac{1}{2\pi} \left( b_1^\parallel \arctan \frac{y}{x} + c_{12} \frac{xy}{r^2} + c_{13} \frac{xy^3}{r^4} \right) \\ u_2 &= \frac{1}{2\pi} \left( -c_{21} \ln \frac{r}{r_0} + c_{22} \frac{y^2}{r^2} + c_{23} \frac{y^2(y^2 - x^2)}{2r^4} \right) \\ u_3 &= \frac{1}{2\pi} \left( -c_{31} \arctan \frac{y}{x} + c_{32} \frac{xy}{r^2} + c_{33} \frac{xy^3}{r^4} \right) \\ w_1 &= \frac{1}{2\pi} \left( b_1^\perp \arctan \frac{y}{x} + c_{42} \frac{xy}{r^2} + c_{43} \frac{xy^3}{r^4} \right) \\ w_2 &= \frac{1}{2\pi} \left( -c_{51} \ln \frac{r}{r_0} + c_{52} \frac{y^2}{r^2} + c_{53} \frac{y^2(y^2 - x^2)}{2r^4} \right) \\ w_3 &= \frac{1}{2\pi} \left( -c_{61} \arctan \frac{y}{x} + c_{62} \frac{xy}{r^2} + c_{63} \frac{xy^3}{r^4} \right) \end{aligned} \tag{14}$$

in which  $r^2 = x^2 + y^2$ ,  $r_0$  is the radius of the dislocation core and  $c_{ij}$  are constants,

$$\begin{aligned} c_{12} &= \frac{2c_0(\mu(2R^2 + c_0\mu)(\lambda^2 + 3\lambda\mu + \mu^2)b_1^\parallel + R(-e(\lambda + \mu) + 2\mu c_0(\lambda + 2\mu)^2)b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{13} &= \frac{2c_0R(\lambda + \mu)(2R\mu(\lambda + \mu)b_1^\parallel + 2\mu c_0(\lambda + 2\mu)b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{21} &= \frac{(2c_0^2\mu^3(\lambda + 2\mu) - 2e^2)b_1^\parallel + 2c_0R(\lambda + 3\mu)eb_1^\perp}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{22} &= \frac{2c_0(-\mu^2(\lambda + \mu)(-2R^2 + c_0(\lambda + 2\mu))b_1^\parallel + R(-(\lambda + \mu)e + 2c_0\mu^2)b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{23} &= \frac{2c_0R(\lambda + \mu)(2R\mu(\lambda + \mu)b_1^\parallel + 2c_0\mu^2b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{31} &= [-3c_1e\{2(c_0\mu + 7e)\mu c_0(\lambda + 2\mu)b_1^\parallel \\ &\quad + R(54c_0^2(\lambda^2 + 3\lambda\mu + \mu^2) - 2(\alpha - \beta)(e + \mu c_0(\lambda + 2\mu)))b_1^\perp\}] \\ &\quad \times [4c_0R(-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu)))]^{-1} \\ c_{32} &= \frac{3c_1e(2\mu(-e + \mu c_0(\lambda + 2\mu))b_1^\parallel + R(-2e + 2\mu c_0(\lambda + 2\mu))b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{33} &= \frac{-3ec_1(2R\mu(\lambda + \mu)b_1^\parallel + 2\mu c_0(\lambda + 2\mu)b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{42} &= \frac{-2e(2R\mu(\lambda + \mu)b_1^\parallel + 2\mu c_0(\lambda + 2\mu)b_1^\perp)}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\ c_{43} &= 0 \end{aligned}$$

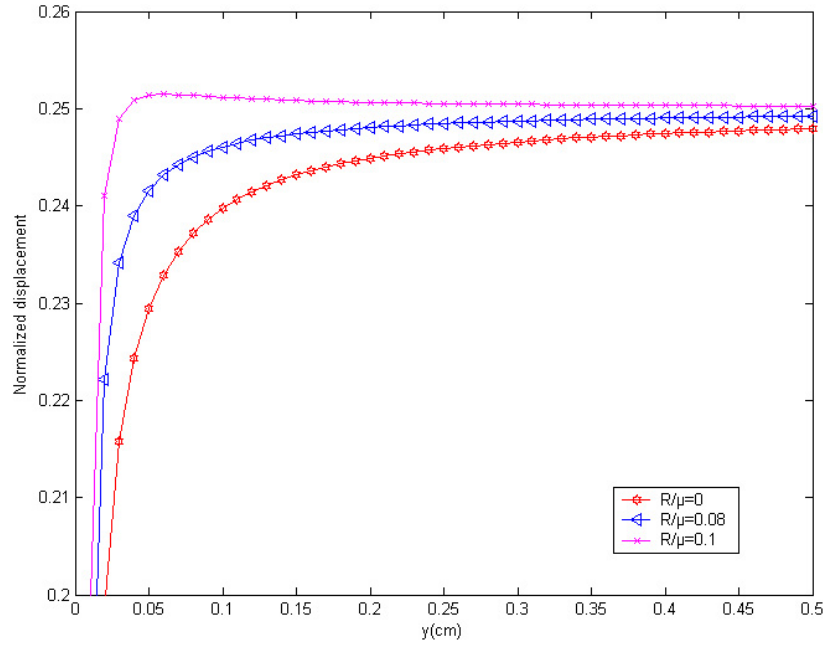


**Figure 1.** The displacement  $u_1/b_1^{\parallel}$  versus  $x$  for different coupling elastic constants.

$$\begin{aligned}
 c_{51} &= -\{-4e\mu^2c_0(\lambda + 2\mu)b_1^{\parallel} + R(2(\lambda + 2\mu)(e + 0.5\mu c_0) + \mu(2\beta^2\mu + 2c_0^2(\lambda + 2\mu)^2 \\
 &\quad + c_0(\lambda + 2\mu)(-\beta\mu + R^2(\lambda + \mu)))b_1^{\perp}\} \\
 &\quad \times \{R(-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu)))\}^{-1} \\
 c_{52} &= -\frac{2e(2R\mu(\lambda + \mu)b_1^{\parallel} + 2\mu c_0(\lambda + 2\mu)b_1^{\perp})}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\
 c_{53} &= 0 \\
 c_{61} &= [-3c_2e\{(2(c_0\mu + 7e)\mu c_0(\lambda + 2\mu)b_1^{\parallel} + R(54c_0^2(\lambda^2 + 3\lambda\mu + \mu^2) \\
 &\quad - 2(\alpha - \beta)(e + \mu c_0(\lambda + 2\mu)))b_1^{\perp}\})] \\
 &\quad \times [4c_0R(-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu)))]^{-1} \\
 c_{62} &= \frac{3ec_2(2\mu(-e + \mu c_0(\lambda + 2\mu))b_1^{\parallel} + R(-2e + 2\mu c_0(\lambda + 2\mu))b_1^{\perp})}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \\
 c_{63} &= \frac{-3ec_2(2R\mu(\lambda + \mu)b_1^{\parallel} + 2\mu c_0(\lambda + 2\mu)b_1^{\perp})}{-e(2e + \mu c_0(\lambda + 2\mu)) + \mu c_0(\lambda + 2\mu)(e + 2\mu c_0(\lambda + 2\mu))} \tag{15}
 \end{aligned}$$

in which  $e = -(\lambda + \mu)R^2$ .

We can see that the phonon–phonon, phason–phason and phonon–phason interaction is very evident, so the solution (14) is quite different from the solution given by Yang *et al* [16] (whose solution for the phonon displacement field is quoted in the following, see formula (17)), where they took  $R = 0$ , i.e., they assumed the phonon and phason are decoupled, so the solution for the phonon is the same as the classic solution for crystals. It is obvious that our solution given by (14) explores the realistic case for quasicrystals, quite different from that of crystals. To illustrate the coupling effect we give some numerical results in figures 1 and 2 for the normalized displacement  $u_1/b_1^{\parallel}$  versus  $x$  and  $y$  respectively, in which the results exhibit the



**Figure 2.** The displacement  $u_1/b_1^{\parallel}$  versus  $y$  for different coupling constants.

influence of parameter  $R$  is significant. In the calculation we take the data of elastic moduli as  $\lambda = 2.3433$ ,  $\mu = 0.5741$ ,  $K_1 = 1.22$ ,  $K_2 = 0.24$  ( $10^{12}$  dyn  $\text{cm}^{-2}$ )

and the phonon–phason coupling elastic constant for three different cases, i.e.  $R/\mu = 0$ ,  $R/\mu = 0.08$  and  $R/\mu = 0.1$ , in which the first one corresponds to the decoupled case. The results are depicted by figure 1 for  $u_1/b_1^{\parallel}$  versus  $x$  and figure 2 for  $u_1/b_1^{\parallel}$  versus  $y$ , respectively.

The figures show that the coupling effect is very important; the displacement is increasing with the growth of value of  $R$ .

For the other two typical problems, in which the Burgers vector of a dislocation is denoted by  $(0, b_2^{\parallel}, 0, 0, b_2^{\perp}, 0)$  and  $(0, 0, b_3^{\parallel}, 0, 0, b_3^{\perp})$  respectively, a complete similar consideration will yield similar results, which are omitted here. Alternatively, the expressions are denoted as  $u_j^{(2)}, w_j^{(2)}$  and  $u_j^{(3)}, w_j^{(3)}$ . Therefore, the explicit analytical expressions for elastic field for a dislocation  $(b_1^{\parallel}, b_2^{\parallel}, b_3^{\parallel}, b_1^{\perp}, b_2^{\perp}, b_3^{\perp})$  in an icosahedral quasicrystal can be obtained by superposition of the corresponding expressions for the elastic fields for  $(b_1^{\parallel}, 0, 0, b_1^{\perp}, 0, 0)$ ,  $(0, b_2^{\parallel}, 0, 0, b_2^{\perp}, 0)$  and  $(0, 0, b_3^{\parallel}, 0, 0, b_3^{\perp})$ , namely

$$u_j = u_j^{(1)} + u_j^{(2)} + u_j^{(3)} \quad w_j = w_j^{(1)} + w_j^{(2)} + w_j^{(3)} \quad i, j = 1, 2, 3. \quad (16)$$

#### 4. Discussion and conclusion

The complete analysis on dislocation of icosahedral quasicrystals has been offered in the previous sections, in which the phonon–phonon, phason–phason and phonon–phason interactions are revealed; in particular, the coupling effect between phonon and phason degrees of freedom has been explored thoroughly. One can see that the interaction is important, which could not be ignored. Of course, the feature of the icosahedral symmetry group which is



infracted by strain and stress tensors and the five independent elastic constants is described by the solution of (14) and (15).

If  $R = 0$ ,  $w_i = 0$ , our solution is exactly reduced to the solution of dislocation of crystals, i.e.

$$\begin{aligned} u_1 &= \frac{b_1^{\parallel}}{2\pi} \left( tg^{-1} \frac{y}{x} + \frac{\lambda + \mu}{\lambda + 2\mu} \frac{xy}{r^2} \right) + \frac{b_2^{\parallel}}{2\pi} \left( \frac{\mu}{\lambda + 2\mu} \ln \frac{r}{r_0} + \frac{\lambda + \mu}{\lambda + 2\mu} \frac{x^2}{r^2} \right) \\ u_2 &= -\frac{b_1^{\parallel}}{2\pi} \left( \frac{\mu}{\lambda + 2\mu} \ln \frac{r}{r_0} + \frac{\lambda + \mu}{\lambda + 2\mu} \frac{x^2}{r^2} \right) + \frac{b_2^{\parallel}}{2\pi} \left( tg^{-1} \frac{y}{x} - \frac{\lambda + \mu}{\lambda + 2\mu} \frac{xy}{r^2} \right) \\ u_3 &= \frac{b_3^{\parallel}}{2\pi} tg^{-1} \frac{y}{x} \end{aligned} \quad (17)$$

which is the well known classical solution. This proves the correctness of our formalism and derivation from one direction.

The displacement potential function formulation proposed by Fan and Guo [17] sets the basis for solving the elasticity and defect problem of icosahedral quasicrystals. The formulation greatly simplifies the solution process. In the subsequent steps a systematic Fourier analysis is developed, which provides a constructed procedure to find the analytic solution; it is effective not only for the dislocation problem, but also for more complicated mixed boundary value problems (e.g. Griffith crack problems); see, e.g., [19]. The present solution is explicit and with closed form.

The present solution can be used as a fundamental solution for a dislocation in an icosahedral quasicrystal. Therefore, many elasticity problems in an icosahedral quasicrystal can be directly solved with the aid of this fundamental solution by superposition.

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## References

- [1] Bak P 1985 *Phys. Rev. Lett.* **54** 1517
- [2] Levine D *et al* 1985 *Phys. Rev. Lett.* **54** 1520
- [3] Socolar J E S, Lubensky T C and Steinhardt P J 1985 *Phys. Rev. Lett.* **54** 1520
- [4] Zhang Z and Urban K 1989 *Phil. Mag. Lett.* **60** 97
- [5] Devaud-Rzepsek J, Cornier-Quiquandon M and Gratias D 1989 *Proc. 3rd Int. Conf. on Quasicrystals and Incommensurate Structures* ed M J Yacamàn, D Romeu, V Castaña and A Gómez (Singapore: World Scientific) p 498
- [6] Ebalard S and Spaepen F 1989 *J. Mater. Res.* **4** 39
- [7] Ding D H *et al* 1993 *Phys. Rev. B* **48** 7003
- [8] Ding D H *et al* 1995 *J. Phys.: Condens. Matter* **7** 5423
- [9] Ding D H *et al* 1995 *Acta Phys. Sin.* **4** 816
- [10] Yang W G *et al* 1995 *Phys. Lett. A* **200** 177
- [11] Qin Y L *et al* 1997 *J. Phys.: Condens. Matter* **9** 859
- [12] Li X F and Fan T Y 1998 *Chin. Phys. Lett.* **15** 278
- [13] Li X *et al* 1999 *J. Phys.: Condens. Matter* **11** 703
- [14] De P and Pelcovits P A 1987 *Phys. Rev. B* **35** 8609
- [15] Fan T Y, Trebin H R, Messerschmit U and Mai Y W 2004 *J. Phys.: Condens. Mater.* **16** 5229
- [16] Yang W G *et al* 1998 *Phil. Mag. A* **77** 1481
- [17] Fan T Y and Guo L H 2005 *Phys. Lett. A* **341** 235
- [18] Bohsung J and Trebin H R 1989 *Introduction to the Mathematics of Quasicrystals* ed M V Jaric (New York: Academic) p 183
- [19] Zhu A Y and Fan T Y 2007 *Chin. Phys.* **16** 1111