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Elastic theory of 1D-quasiperiodic stacking of 2D crystals

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Abstract. A general solution of the elastic fields in 1D hexagonal quasicrystals with point groups $6mm$, 62_h2_h, $\overline{6}m2_h$ and $6/m_hmm$ is given in terms of four 'harmonic' functions F_i $(i = 1, 2, 3, 4)$. Then we consider the problem of a circular crack embedded in an infinite 1D hexagonal quasicrystal of point group $6mm$. The results obtained in this paper automatically reduce to those in the classical elasticity theory when the phason field is absent.

1. Introduction

A one-dimensional (1D) quasicrystal (QC) refers to a three-dimensional (3D) solid structure with periodic arrangement in a plane and quasiperiodic arrangement in the third direction. So far two kinds of 1D QC have been discovered and studied. Merlin *et al* [1], Hu *et al* [2], Feng *et al* [3], Terauchi *et al* [4] and Chen *et al* [5, 6] prepared a Fibonacci sequence with alternating layers of GaAs and AlAs or $Al_{0.5}Ga_{0.5}As$, where the GaAs and AlAs were grown by molecular-beam epitaxy. He *et al* [7] found a 1D QC derived from the 2D decagonal QC in rapidly solidified Al–Ni–Si, Al–Cu–Mn and Al–Cu–Co alloys. Tsai *et al* [8] and Yang *et al* [9] reported the discovery of some stable 1D QCs in the Al–Cu–Fe–Mn system. Recently, Wang *et al* [10] derived all 31 possible 1D QC point groups, which can be divided into ten Laue classes and six 1D QC systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal and hexagonal systems, and obtained a generalized Hooke law of a 1D QC. On the other hand, as in conventional crystals, many structural defects have already been observed experimentally in QCs and experiments show that the QCs are quite brittle. So the defect problems for QCs, such as dislocation and crack problems, are studied by many authors [11–16]. However, most of the studies are made under the assumption that the elastic field induced in QCs is independent of the variable z. In other words, they consider only the elastic plane or antiplane problems for QCs because of the complexities of the problems.

In the present paper, a general solution of the elastic fields in 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\overline{6}m2_h$ and $6/m_hmm$ is given in terms of four 'harmonic' functions F_i $(i = 1, 2, 3, 4)$. To illustrate the utility of the general solution, we consider the problem of a circular crack embedded in an infinite 1D hexagonal QC of point group $6mm$. The stresses and displacements in the whole QC and the mode I stress intensity factor (SIF) on the front of the circular crack are given. All the results obtained in this paper automatically reduce to those in the classical elasticity theory when the phason field is absent.

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2. The general solution of the elastic field in 1D hexagonal QCs

According to 1D QC elasticity theory [10], strain– and stress–displacement relations for 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$, respectively, are

$$
\begin{aligned}
&\varepsilon_{ij} = (\partial_j u_i + \partial_i u_j)/2 \qquad w_{ij} = \partial_j w_i \\
&\sigma_{xx} = c_{11}\partial_x u_x + (c_{11} - 2c_{66})\partial_y u_y + c_{13}\partial_z u_z + R_1\partial_z w_z \\
&\sigma_{yy} = (c_{11} - 2c_{66})\partial_x u_x + c_{11}\partial_y u_y + c_{13}\partial_z u_z + R_1\partial_z w_z \\
&\sigma_{zz} = c_{13}\partial_x u_x + c_{13}\partial_y u_y + c_{33}\partial_z u_z + R_2\partial_z w_z \\
&\sigma_{yz} = \sigma_{zy} = c_{44}(\partial_y u_z + \partial_z u_y) + R_3\partial_y w_z \\
&\sigma_{zx} = \sigma_{xz} = c_{44}(\partial_x u_z + \partial_z u_x) + R_3\partial_x w_z \\
&\sigma_{xy} = \sigma_{yx} = c_{66}(\partial_x u_y + \partial_y u_x) \\
&H_{zz} = R_1(\partial_x u_x + \partial_y u_y) + R_2\partial_z u_z + K_1\partial_z w_z \\
&H_{zx} = R_3(\partial_x u_z + \partial_z u_x) + K_2\partial_x w_z \\
&H_{zy} = R_3(\partial_y u_z + \partial_z u_y) + K_2\partial_y w_z.
\end{aligned}
\tag{1}
$$

The equilibrium equations, in the absence of body forces, are

$$
\begin{aligned}
&\partial_x\sigma_{xx} + \partial_y\sigma_{xy} + \partial_z\sigma_{xz} = 0 \\
&\partial_x\sigma_{yx} + \partial_y\sigma_{yy} + \partial_z\sigma_{yz} = 0 \\
&\partial_x\sigma_{zx} + \partial_y\sigma_{zy} + \partial_z\sigma_{zz} = 0 \\
&\partial_x H_{zx} + \partial_y H_{zy} + \partial_z H_{zz} = 0
\end{aligned}
\tag{2}
$$

where the z-axis is assumed to be the quasiperiodic axis, and the xy-plane the periodic plane of the QC, u_i, w_i phonon and phason displacements in the physical and perpendicular spaces, respectively, σ_{ij} and ε_{ij} phonon stresses and strains, H_{ij} and w_{ij} phason stresses and strains, c_{11}, c_{13}, c_{33}, c_{44}, c_{66}, K_1, K_2 the elastic constants corresponding to the phonon and phason fields and R_1, R_2, R_3 the elastic constants of phonon–phason coupling. We should keep in mind that the subscripts i, j for H_{ij}, w_{ij} cannot be exchanged according to their meanings [17]. It is very important for us to write the boundary conditions correctly.

The substitution of (1) into (2) gives

$$
\begin{aligned}
&(c_{11}\partial_x^2 + c_{66}\partial_y^2 + c_{44}\partial_z^2)u_x + (c_{11} - c_{66})\partial_x\partial_y u_y + (c_{13} + c_{44})\partial_x\partial_z u_z + (R_1 + R_3)\partial_x\partial_z w_z = 0 \\
&(c_{11} - c_{66})\partial_x\partial_y u_x + (c_{66}\partial_x^2 + c_{11}\partial_y^2 + c_{44}\partial_z^2)u_y + (c_{13} + c_{44})\partial_y\partial_z u_z + (R_1 + R_3)\partial_y\partial_z w_z = 0 \\
&(c_{13} + c_{44})(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + (c_{44}\partial_x^2 + c_{44}\partial_y^2 + c_{33}\partial_z^2)u_z + [R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]w_z = 0 \\
&(R_1 + R_3)(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + [R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]u_z + [K_2(\partial_x^2 + \partial_y^2) + K_1\partial_z^2]w_z = 0.
\end{aligned}
\tag{3}
$$

One can directly verify that equations (3) can be satisfied by

$$
\begin{aligned}
&u_x = \partial_x(F_1 + F_2 + F_3) - \partial_y F_4 \qquad u_y = \partial_y(F_1 + F_2 + F_3) + \partial_x F_4 \\
&u_z = \partial_z(m_1F_1 + m_2F_2 + m_3F_3) \qquad w_z = \partial_z(l_1F_1 + l_2F_2 + l_3F_3)
\end{aligned}
\tag{4}
$$

where the possible functions F_i are the solutions of

$$
(\partial_x^2 + \partial_y^2 + \gamma_i^2\partial_z^2)F_i = 0 \qquad i = 1, 2, 3, 4 \tag{5}
$$

where the values of m_i, l_i and γ_i are related by the following expressions:

$$
\begin{aligned}
\frac{c_{44} + (c_{13} + c_{44})m_i + (R_1 + R_3)l_i}{c_{11}} &= \frac{c_{33}m_i + R_2l_i}{c_{13} + c_{44} + c_{44}m_i + R_3l_i} \\
&= \frac{R_2m_i + K_1l_i}{R_1 + R_3 + R_3m_i + K_2l_i} = \gamma_i^2 \qquad i = 1, 2, 3 \qquad c_{44}/c_{66} = \gamma_4^2.
\end{aligned}
\tag{6}
$$

Note that we use γ_i^2 in place of γ_i for convenience as in [18]. The expressions (6) are the exact analogues of those used by Fabrikant [18] and Elliott [19] for aeolotropic hexagonal crystals and in fact can reduce to those when the phason field is absent.

Substituting (4) into (1), and using (5), we have

$$\begin{aligned}
\sigma_{xx} &= [c_{11}\partial_x^2 + (c_{11} - 2c_{66})\partial_y^2](F_1 + F_2 + F_3) - 2c_{66}\partial_x\partial_y F_4 \\
&\quad + c_{13}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) + R_1\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{yy} &= [(c_{11} - 2c_{66})\partial_x^2 + c_{11}\partial_y^2](F_1 + F_2 + F_3) + 2c_{66}\partial_x\partial_y F_4 \\
&\quad + c_{13}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) + R_1\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{zz} &= -c_{13}\partial_z^2(\gamma_1^2F_1 + \gamma_2^2F_2 + \gamma_3^2F_3) + c_{33}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) \\
&\quad + R_2\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{xy} &= \sigma_{yx} = 2c_{66}\partial_x\partial_y(F_1 + F_2 + F_3) + c_{66}(\partial_x^2 - \partial_y^2)F_4 \\
\sigma_{yz} &= \sigma_{zy} = c_{44}\partial_y\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad + c_{44}\partial_x\partial_z F_4 + R_3\partial_y\partial_z(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{zx} &= \sigma_{xz} = c_{44}\partial_x\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad - c_{44}\partial_y\partial_z F_4 + R_3\partial_x\partial_z(l_1F_1 + l_2F_2 + l_3F_3) \\
H_{zz} &= -R_1\partial_z^2(\gamma_1^2F_1 + \gamma_2^2F_2 + \gamma_3^2F_3) + R_2\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) \\
&\quad + K_1\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
H_{zx} &= R_3\partial_x\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad - R_3\partial_y\partial_z F_4 + K_2\partial_x\partial_z(l_1F_1 + l_2F_2 + l_3F_3) \\
H_{zy} &= R_3\partial_y\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad + R_3\partial_x\partial_z F_4 + K_2\partial_y\partial_z(l_1F_1 + l_2F_2 + l_3F_3).
\end{aligned} \tag{7}$$

In cylindrical polar coordinates, the governing equations (5) are

$$(\partial_r^2 + 1/r\partial_r + 1/r^2\partial_\theta^2 + \gamma_i^2\partial_z^2)F_i = 0 \qquad i = 1, 2, 3, 4 \tag{8}$$

and the general solutions (4) and (7) are given by

$$\begin{aligned}
u_r &= \partial_r(F_1 + F_2 + F_3) - 1/r\partial_\theta F_4 \qquad & u_\theta &= 1/r\partial_\theta(F_1 + F_2 + F_3) + \partial_r F_4 \\
u_z &= \partial_z(m_1F_1 + m_2F_2 + m_3F_3) \qquad & w_z &= \partial_z(l_1F_1 + l_2F_2 + l_3F_3)
\end{aligned} \tag{9}$$

$$\begin{aligned}
\sigma_{rr} &= [c_{11}\partial_r^2 + (c_{11} - 2c_{66})(1/r\partial_r + 1/r^2\partial_\theta^2)](F_1 + F_2 + F_3) \\
&\quad + c_{13}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) - 2c_{66}(1/r\partial_r\partial_\theta - 1/r^2\partial_\theta)F_4 \\
&\quad + R_1\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{\theta\theta} &= [(c_{11} - 2c_{66})\partial_r^2 + c_{11}(1/r\partial_r + 1/r^2\partial_\theta^2)](F_1 + F_2 + F_3) \\
&\quad + c_{13}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) + 2c_{66}(1/r\partial_r\partial_\theta - 1/r^2\partial_\theta)F_4 \\
&\quad + R_1\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{zz} &= -c_{13}\partial_z^2(\gamma_1^2F_1 + \gamma_2^2F_2 + \gamma_3^2F_3) + c_{33}\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3) \\
&\quad + R_2\partial_z^2(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{r\theta} &= \sigma_{\theta r} = 2c_{66}(1/r\partial_r\partial_\theta - 1/r^2\partial_\theta)(F_1 + F_2 + F_3) + c_{66}(\partial_r^2 - 1/r\partial_r - 1/r^2\partial_\theta^2)F_4 \\
\sigma_{\theta z} &= \sigma_{z\theta} = c_{44}1/r\partial_\theta\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad + c_{44}\partial_r\partial_z F_4 + R_3 1/r\partial_\theta\partial_z(l_1F_1 + l_2F_2 + l_3F_3) \\
\sigma_{zr} &= \sigma_{rz} = c_{44}\partial_r\partial_z[(m_1+1)F_1 + (m_2+1)F_2 + (m_3+1)F_3] \\
&\quad - c_{44}1/r\partial_\theta\partial_z F_4 + R_3\partial_r\partial_z(l_1F_1 + l_2F_2 + l_3F_3) \\
H_{zz} &= -R_1\partial_z^2(\gamma_1^2F_1 + \gamma_2^2F_2 + \gamma_3^2F_3) + R_2\partial_z^2(m_1F_1 + m_2F_2 + m_3F_3)
\end{aligned} \tag{10}$$

$$
\begin{aligned}
&+K_1\partial_z^2(l_1F_1+l_2F_2+l_3F_3)\\
H_{zr} &= R_3\partial_r\partial_z[(m_1+1)F_1+(m_2+1)F_2+(m_3+1)F_3]\\
&\quad -R_3 1/r\partial_\theta\partial_zF_4+K_2\partial_r\partial_z(l_1F_1+l_2F_2+l_3F_3)\\
H_{z\theta} &= R_3 1/r\partial_\theta\partial_z[(m_1+1)F_1+(m_2+1)F_2+(m_3+1)F_3]\\
&\quad +R_3\partial_r\partial_zF_4+K_2 1/r\partial_\theta\partial_z(l_1F_1+l_2F_2+l_3F_3).
\end{aligned}
$$

3. The effect of a crack in an infinite 1D hexagonal QC

In the above, we have discussed the general solution of 3D elastic problems for 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$ and found that a solution was possible in terms of four functions F_i ($i = 1,2,3,4$). In the following, we consider an infinite 1D hexagonal QC of point group $6mm$ weakened by a flat circular crack with radius a in the plane $z = 0$, with uniform loads applied normal to the crack faces. Due to symmetry, the problem can be formulated as follows: find the solution to the set of differential equations (8) for a half-space $z \geqslant 0$, subject to the mixed boundary conditions in the plane $z = 0$

$$
\begin{array}{lll}
\sigma_{zz} = -\sigma & H_{zz} = -\tau & 0 < r < a\\
u_z = 0 & w_z = 0 & r > a\\
\sigma_{zr} = 0 & \sigma_{z\theta} = 0 & r \geqslant 0.
\end{array}
\tag{11}
$$

Note that cylindrical polar coordinates in this case have been used, and we suppose the elastic field under this loading condition to be independent of θ. We should also note that $H_{rz} = H_{\theta z} = 0$ for $r \geqslant 0$ is satisfied. After the Hankel transformation to equation (8), considering the boundary condition at infinity:

$$
\sigma_{ij} \to 0 \qquad H_{ij} \to 0 \qquad \sqrt{r^2+z^2} \to \infty \tag{12}
$$

the solution of (8) can be expressed as:

$$
F_i(r,z) = \int_0^\infty \xi A_i(\xi)\exp(-\xi z/\gamma_i)J_0(\xi r)\,\mathrm{d}\xi \qquad i = 1,2,3,4. \tag{13}
$$

We now show that such a solution can in fact satisfy all our boundary conditions for our problems. It follows from $\sigma_{z\theta} = 0$ for $r \geqslant 0$ that $F_4 = 0$. From $\sigma_{zz} = 0$ for $r \geqslant 0$, we have

$$
A_3 = -\left[\frac{R_3l_1+c_{44}(1+m_1)}{\gamma_1}A_1+\frac{R_3l_2+c_{44}(1+m_2)}{\gamma_2}A_2\right]\frac{\gamma_3}{R_3l_3+c_{44}(1+m_3)}. \tag{14}
$$

According to the rest of the boundary conditions (11) and expressions (9), (10) and (14), we get

$$
\begin{cases}
\displaystyle\int_0^\infty \xi^3A_1(\xi)J_0(\xi r)\,\mathrm{d}\xi = (c_2\sigma - c_4\tau)/(c_1c_4-c_2c_3) & 0 < r < a\\
\displaystyle\int_0^\infty \xi^2A_1(\xi)J_0(\xi r)\,\mathrm{d}\xi = 0 & r > a
\end{cases}
\tag{15}
$$

$$
\begin{cases}
\displaystyle\int_0^\infty \xi^3A_2(\xi)J_0(\xi r)\,\mathrm{d}\xi = (c_1\sigma - c_3\tau)/(c_2c_3-c_1c_4) & 0 < r < a\\
\displaystyle\int_0^\infty \xi^2A_2(\xi)J_0(\xi r)\,\mathrm{d}\xi = 0 & r > a
\end{cases}
\tag{16}
$$

with

$$
c_i = \frac{R_2m_i+K_1l_i-R_1\gamma_i^2}{\gamma_i^2} - \frac{[R_3l_i+c_{44}(1+m_i)][R_2m_3+K_1l_3-R_1\gamma_3^2]}{\gamma_i\gamma_3[R_3l_3+c_{44}(1+m_3)]} \qquad i = 1,2
$$

$$c_{j+2} = \frac{c_{33}m_j + R_2 l_j - c_{13}\gamma_j^2}{\gamma_j^2} - \frac{[R_3 l_j + c_{44}(1+m_j)][c_{33}m_3 + R_2 l_3 - c_{13}\gamma_3^2]}{\gamma_j\gamma_3[R_3 l_3 + c_{44}(1+m_3)]} \qquad j = 1, 2.$$

It follows from (15) and (16) that (see appendix)

$$\begin{aligned} A_1(\xi) &= [2(c_2\sigma - c_4\tau)/\pi(c_1c_4 - c_2c_3)]\xi^{-3}(\xi^{-1}\sin a\xi - a\cos a\xi) \\ A_2(\xi) &= [2(c_1\sigma - c_3\tau)/\pi(c_2c_3 - c_1c_4)]\xi^{-3}(\xi^{-1}\sin a\xi - a\cos a\xi). \end{aligned} \tag{17}$$

From (9), (10), (13), (14) and (17), the stresses and displacements in the whole QC are given as follows:

$$\begin{aligned}
\sigma_{rr} &= \sum_{i=1}^{3}\frac{-c_{11}\gamma_i^2 + c_{13}m_i + R_1 l_i}{\gamma_i^2} a_i[S_0^0(\rho, z_i) - C_2^0(\rho, z_i)] \\
&\qquad + 2c_{66}\frac{a}{r}\sum_{i=1}^{3} a_i[S_{-1}^1(\rho, z_i) - C_1^1(\rho, z_i)] \\
\sigma_{\theta\theta} &= \sum_{i=1}^{3}\frac{-c_{11}\gamma_i^2 + c_{13}m_i + R_1 l_i}{\gamma_i^2} a_i[S_0^0(\rho, z_i) - C_2^0(\rho, z_i)] \\
&\qquad + 2c_{66}\sum_{i=1}^{3} a_i\left\{S_0^0(\rho, z_i) - C_2^0(\rho, z_i) - \frac{a}{r}[S_{-1}^1(\rho, z_i) - C_1^1(\rho, z_i)]\right\} \\
\sigma_{zz} &= \sum_{i=1}^{3}\frac{-c_{13}\gamma_i^2 + c_{33}m_i + R_2 l_i}{\gamma_i^2} a_i[S_0^0(\rho, z_i) - C_2^0(\rho, z_i)] \\
\sigma_{zr} = \sigma_{rz} &= \sum_{i=1}^{3}\frac{c_{44}(m_i+1) + R_3 l_i}{\gamma_i} a_i[S_0^1(\rho, z_i) - C_2^1(\rho, z_i)] \\
H_{zz} &= \sum_{i=1}^{3}\frac{-R_1\gamma_i^2 + R_2 m_i + K_1 l_i}{\gamma_i^2} a_i[S_0^0(\rho, z_i) - C_2^0(\rho, z_i)] \\
H_{zr} &= \sum_{i=1}^{3}\frac{R_3(m_i+1) + K_2 l_i}{\gamma_i} a_i[S_0^1(\rho, z_i) - C_2^1(\rho, z_i)] \\
u_r &= -a\sum_{i=1}^{3} a_i[S_{-1}^1(\rho, z_i) - C_1^1(\rho, z_i)] \\
u_z &= -a\sum_{i=1}^{3}\frac{m_i}{\gamma_i} a_i[S_{-1}^0(\rho, z_i) - C_1^0(\rho, z_i)] \\
w_z &= -a\sum_{i=1}^{3}\frac{l_i}{\gamma_i} a_i[S_{-1}^0(\rho, z_i) - C_1^0(\rho, z_i)] \\
\sigma_{r\theta} &= \sigma_{\theta r} = 0 \qquad \sigma_{z\theta} = \sigma_{\theta z} = 0 \qquad H_{z\theta} = 0 \qquad u_\theta = 0
\end{aligned} \tag{18}$$

where

$$a_1 = \frac{2(c_2\sigma - c_4\tau)}{\pi(c_1c_4 - c_2c_3)} \qquad a_2 = \frac{2(c_1\sigma - c_3\tau)}{\pi(c_2c_3 - c_1c_4)} \qquad a_3 = b_1a_1 + b_2a_2$$

$$b_i = -\frac{R_3 l_i + c_{44}(1+m_i)}{\gamma_i}\frac{\gamma_3}{R_3 l_3 + c_{44}(1+m_3)} \qquad i = 1, 2$$

$$S_n^m(\rho, z) = \int_0^\infty \eta^{n-1}\sin\eta\, \mathrm{e}^{-\eta z} J_m(\eta\rho)\,\mathrm{d}\eta \qquad C_n^m(\rho, z) = \int_0^\infty \eta^{n-2}\cos\eta\, \mathrm{e}^{-\eta z} J_m(\eta\rho)\,\mathrm{d}\eta$$

$$\eta = a\xi \qquad z_i = z/(\gamma_i a) \qquad \rho = r/a.$$

These integrals may be evaluated by methods given by Watson [20]. In the following we calculate the most important physical quantity in fracture theory—the stress intensity factor.

As in the elastic plane or antiplane problems for QCs [13, 14], we define

$$K_1^{\Pi} = \lim_{r\to a+} \sqrt{2\pi(r-a)}\sigma_{zz}(r,0). \tag{19}$$

It follows from (18) that

$$\sigma_{zz}(r,0) = \begin{cases} -\sigma & 0<r<a \\ -\dfrac{2\sigma}{\pi}\left(\arcsin\dfrac{a}{r} - \dfrac{a}{\sqrt{r^2-a^2}}\right) & r>a \end{cases} \tag{20}$$

$$H_{zz}(r,0) = \begin{cases} -\tau & 0<r<a \\ -\dfrac{2\tau}{\pi}\left(\arcsin\dfrac{a}{r} - \dfrac{a}{\sqrt{r^2-a^2}}\right) & r>a. \end{cases} \tag{21}$$

The substitution of (20) into (19) yields

$$K_1^{\Pi} = 2\sqrt{a/\pi}\sigma.$$

The SIF is independent of the elastic constants, which is in accordance with elastic plane and antiplane problems in QCs [13, 14].

4. Discussion and conclusions

The elastic 3D problems for 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\overline{6}m2_h$ and $6/m_hmm$ are studied, and solutions are found in terms of four 'harmonic' functions F_i ($i = 1, 2, 3, 4$). The solutions for aeolotropic hexagonal crystals can be deduced as a special case. The SIF for mode I in a cracked 1D hexagonal QC of point group $6mm$ is independent of elastic constants, which is identical with the corresponding result in conventional linear elasticity fracture mechanics [21]. It is of interest to note that the stress component $H_{zz}(r, 0)$ of the phason field also exhibits the square root singularity on the front of the crack (see (21)). If we further extend the SIF for the photon field to the phason field, defining:

$$K_1^{\perp} = \lim_{r\to a+} \sqrt{2\pi(r-a)}H_{zz}(r,0) \tag{22}$$

then substituting (21) into (22), we have

$$K_1^{\perp} = 2\sqrt{a/\pi}\tau$$

which is also independent of elastic constants. Thus it may be predicted that the basic criteria of fracture based on the fundamentals of conventional linear elasticity fracture mechanics are no longer suitable for QCs.

On the other hand, we have not imposed any restriction on the reality of our solutions, and also not discussed the nature of the values of l_i and m_i ($i = 1, 2, 3$), which themselves affect the reality of the solutions. To the present authors' knowledge, although the phonon elastic constants in QCs can be measured by some experimental methods, the phason and phonon–phason coupling elastic constants are difficult to measure [22]. Up to now, the relevant data, such as constants K_1, K_2, R_1, R_2 and R_3, associated with the present paper are still lacking. Therefore, the equations and solutions derived here by an analytical approach provide only a theoretical model.

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Appendix

Equations of the type

$$\begin{cases} \int_0^\infty y f(y) J_0(xy)\,\mathrm{d}y = g(x) & 0 < x < 1 \\ \int_0^\infty f(y) J_0(xy)\,\mathrm{d}y = 0 & x > 1 \end{cases} \tag{A1}$$

are called dual integral equations and may be solved by the Mellin transform. According to the theory of dual integral equations [23, 24], the solution of equation (A1) reads

$$f(x) = \frac{2}{\pi}\int_0^1 \eta \sin\eta x\,\mathrm{d}\eta \int_0^1 g(\eta\zeta)\zeta(1-\zeta^2)^{-\frac{1}{2}}\,\mathrm{d}\zeta. \tag{A2}$$

When $G(x) \equiv G$ (constant), we have

$$f(x) = \frac{2G}{\pi}x^{-1}(x^{-1}\sin x - \cos x). \tag{A3}$$

In (15), let $r/a = x$, $\xi a = y$, we get (A1) with

$$f(y) = y^2 A_1\left(\frac{y}{a}\right) \qquad g(x) = G = [(c_2\sigma - c_4\tau)/(c_1c_4 - c_2c_3)]a^4.$$

Thus, according to (A3), we can easily obtain the first of equation (17), and the second can also be obtained by the same procedure.

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