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Elastic analysis of a mode II crack in an icosahedral quasicrystal*

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Based on the displacement potential functions, the elastic analysis of a mode II crack in an icosahedral quasicrystal is performed by using the Fourier transform and dual integral equation theory. By the solution, the analytic expressions for the displacement field and stress field are obtained. The asymptotic behaviours of the phonon and phason stress fields around the crack tip indicate that the stresses near the crack tip exhibit a square root singularity. The most important physical quantities of fracture theory, crack stress intensity factor and energy release rate, are evaluated in an explicit version.

Keywords: icosahedral quasicrystal, elasticity, crack, energy release rate
PACC: 6140M, 4630C, 4630N

1. Introduction

Quasicrystals (solids with a long-range orientational order and a long-range quasiperiodic translational order) [1] have become one of topics of the theoretical and experimental studies in the physics of condensed matter. Since the first discovery of icosahedral quasicrystals in Al–Mn alloys,[2] the physical properties, such as the mechanical, electronic, magnetic, optical and thermal properties of quasicrystals have been investigated intensively. Elasticity is one of important properties of quasicrystals. Within the framework of the Landau theory, Bak [3,4] and Levine *et al*[5] formulated the elastic energy of the quasicrystals. Later on, Ding *et al*[6] established the generalized linear elasticity theory of quasicrystals. Lubensky *et al*[7] suggested the hydrodynamics equations of the material. Since quasicrystals are brittle solids at room temperature,[8] it is appropriate to adopt linear elasticity theory to analyse their mechanical property.

In the investigation of dislocations in quasicrystals, Levine *et al*[5] and Socolar *et al*[9] predicted the existence of dislocation and established dislocation theory before their observation experimentally.[10,11] Soon after, the analytical expressions for the displacement field and stress field induced by a dislocation in several quasicrystals were derived by De and Pecovits,[12] Ding *et al*,[13,14] Qin *et al*,[15] Yang *et al*,[16−18] Hu *et al*,[19,20] Fan *et al*,[21−23] and Li *et al*.[24] Some further discussion on energies of dislocations and dislocation dissociation was given by Wollgarten *et al*.[25]

Recently, some experimental evidence has revealed that some two-dimensional detects such as planar defects and cracks caused by cleavage are defective in quasicrystals.[26−32] These macroscopic defects influence strongly the mechanical properties of quasicrystals such as fracture toughness, fracture strength, etc. Since the introduction of the phason field in quasicrystals, their fracture behaviour has presented quite different characters from those of crystals. Some characteristics related to the phason field of crack propagation in a quasicrystal have been pointed out by Mikulla *et al*[33] by molecular dynamics simulation. Therefore, to quantitatively describe the influence of cracks on the mechanical behaviour of quasicrystals, fracture mechanics in quasicrystals, including the determination of the elastic field, the energy release rate and so forth, is a prerequisite. Some other relevant discussions about quasicrystals are given in Refs.[34–37].

Up to now the observed individual quasicrystals are over 200 varieties; among them there are 96 varieties of icosahedral quasicrystals and 65 varieties of decagonal ones. This shows that the icosahedral qua-

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sicrystals play a central role in the materials. Icosahedral quasicrystal is a three-dimensional one, with a huge number of field variables and field equations involving the elasticity. Since the discovery there has been no analytic solution for the crack for icosahedral quasicrystal. The observation of exact analytic solution is of great importance.

Because of the importance of dislocations and dislocation motion to the elasticity and plasticity of the material, and the inherent connection between dislocations and a mode II crack, in this paper we are concerned with a mode II crack in an icosahedral quasicrystal. Based on a general solution in terms of the displacement function G, a mixed boundary value problem is reduced to solving dual integral equations. By solving the resulting equations, the analytic expressions for the displacement field and the singular behaviour of the stress field around a crack tip are explored and determined. Moreover, the stress intensity factor and the energy release rate for the crack tip are given.

2. Simplification of the basic equations

According to the description of an 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 is three-dimensional physical or parallel space, $E_{\parallel}$, and the other is n-dimensional perpendicular or complementary space, $E_{\perp}$. Therefore, for each quasicrystal, in addition to the usual phonon displacements u_i and phonon strains ε_{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 section, we consider a three-dimensional icosahedral quasicrystal with a mode II Griffith crack along the x_3-axis. It is obvious that elastic field induced by a uniform shear stress at infinity is independent of x_3, i.e. the field variables are independent of x_3 or $\partial/\partial x_3 = 0$. In this case, the generalized Hooke law is as follows:[6]

$$\begin{aligned} \sigma_{ij} &= C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl}, \\ H_{ij} &= R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl}, \end{aligned} \tag{1}$$

in which σ_{ij} and H_{ij} are phonon and phason stress tensors, and

$$\varepsilon_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big),$$

$$w_{ij} = \frac{\partial w_i}{\partial x_j},$$

C_{ijkl} and K_{ijkl} the elastic constants of phonon and the phason field respectively, and R_{ijkl} the phonon–phason coupling elastic constants. If the coordinate system can be chosen, with the x_3-axis pointing forwards a vertex of an icosahedral quasicrystal, then there exist

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{2}$$

and $[K]$ and $[R]$ which are expressed as follows:

$$[K] = \begin{bmatrix} K_1 & 0 & 0 & 0 & K_2 & 0 & 0 & K_2 & 0 \\ 0 & K_1 & 0 & 0 & -K_2 & 0 & 0 & K_2 & 0 \\ 0 & 0 & K_2+K_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_1-K_2 & 0 & K_2 & 0 & 0 & -K_2 \\ K_2 & -K_2 & 0 & 0 & K_1-K_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & K_2 & 0 & K_1 & -K_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -K_2 & K_1-K_2 & 0 & -K_2 \\ K_2 & K_2 & 0 & 0 & 0 & 0 & 0 & K_1-K_2 & 0 \\ 0 & 0 & 0 & -K_2 & 0 & 0 & -K_2 & 0 & K_1 \end{bmatrix},$$

$$[R]=R\begin{bmatrix}1&1&1&0&0&0&0&1&0\\-1&-1&1&0&0&0&0&-1&0\\0&0&-2&0&0&0&0&0&0\\0&0&0&0&0&-1&1&0&-1\\1&-1&0&0&1&0&0&0&0\\0&0&0&-1&0&-1&0&0&1\\0&0&0&0&0&-1&1&0&-1\\1&-1&0&0&1&0&0&0&0\\0&0&0&-1&0&-1&0&0&1\end{bmatrix}, \tag{3}$$

where λ and μ are the Lamé constants of the material.

According to the above-mentioned $\partial/\partial x_3=0$, the governing equations of plane elasticity problems for the x_1x_2 plane in an icosahedral quasicrystal are[6,23]

$$\begin{aligned}
&\mu\nabla^2u_1+(\lambda+\mu)\frac{\partial}{\partial x_1}\nabla\cdot\boldsymbol{u}+R\Big(\frac{\partial^2w_1}{\partial x_1^2}+2\frac{\partial^2w_2}{\partial x_1\partial x_2}-\frac{\partial^2w_1}{\partial x_2^2}\Big)=0,\\
&\mu\nabla^2u_2+(\lambda+\mu)\frac{\partial}{\partial x_2}\nabla\cdot\boldsymbol{u}+R\Big(\frac{\partial^2w_2}{\partial x_1^2}-2\frac{\partial^2w_1}{\partial x_1\partial x_2}-\frac{\partial^2w_2}{\partial x_2^2}\Big)=0,\\
&\mu\nabla^2u_3+R\Big(\frac{\partial^2w_1}{\partial x_1^2}-2\frac{\partial^2w_2}{\partial x_1\partial x_2}-\frac{\partial^2w_1}{\partial x_2^2}+\nabla^2w_3\Big)=0,\\
&K_1\nabla^2w_1+K_2\Big(\frac{\partial^2w_3}{\partial x_1^2}-\frac{\partial^2w_3}{\partial x_2^2}\Big)+R\Big(\frac{\partial^2u_1}{\partial x_1^2}-2\frac{\partial^2u_2}{\partial x_1\partial x_2}-\frac{\partial^2u_1}{\partial x_2^2}+\frac{\partial^2u_3}{\partial x_1^2}-\frac{\partial^2u_3}{\partial x_2^2}\Big)=0,\\
&K_1\nabla^2w_2-2K_2\frac{\partial^2w_3}{\partial x_1\partial x_2}+R\Big(\frac{\partial^2u_2}{\partial x_1^2}+2\frac{\partial^2u_1}{\partial x_1\partial x_2}-\frac{\partial^2u_2}{\partial x_2^2}-2\frac{\partial^2u_3}{\partial x_1\partial x_2}\Big)=0,\\
&(K_1-K_2)\nabla^2w_3+K_2\Big(\frac{\partial^2w_1}{\partial x_1^2}-2\frac{\partial^2w_2}{\partial x_1\partial x_2}-\frac{\partial^2w_1}{\partial x_2^2}\Big)+R\nabla^2u_3=0,
\end{aligned} \tag{4}$$

in which $\boldsymbol{u}=(u_1,u_2,u_3)$.

As a result, the key of the task is to determine the elastic field in the x_1x_2 plane, in order to solve plane elasticity problems of an icosahedral quasicrystal. It is convenient to employ the formula obtained previously by Fan and Guo,[23] but some description needs to be added, that is, for a plane elasticity problem in the x_1x_2 plane of an icosahedral quasicrystal, the phonon and phason displacement that can be expressed in terms of $G(x_1,x_2)$, the displacement potential function, as follows:

$$\begin{aligned}
u_1=&R\frac{\partial^2}{\partial x_1\partial x_2}\nabla^2\nabla^2[\mu\alpha\Pi_1+\beta(\lambda+2\mu)\Pi_2]G\\
&+c_0R\frac{\partial^2}{\partial x_1\partial x_2}\Lambda\Big[(3\mu-\lambda)\frac{\partial^4}{\partial x_1^4}+10(\lambda+\mu)\frac{\partial^4}{\partial x_1^2\partial x_2^2}-(5\lambda+9\mu)\frac{\partial^4}{\partial x_2^4}\Big]G,\\
u_2=&R\nabla^2\nabla^2\Big[\mu\alpha\frac{\partial^2}{\partial x_2^2}\Pi_1-\beta(\lambda+2\mu)\frac{\partial^2}{\partial x_1^2}\Pi_2\Big]G\\
&+c_0R\Lambda^2\Big[(\lambda+2\mu)\frac{\partial^6}{\partial x_1^6}-5(2\lambda+3\mu)\frac{\partial^6}{\partial x_1^4\partial x_2^2}+5\lambda\frac{\partial^6}{\partial x_1^2\partial x_2^4}+\mu\frac{\partial^6}{\partial x_2^6}\Big]G,\\
u_3=&c_1\frac{\partial^2}{\partial x_1\partial x_2}\Big[(\alpha-\beta)\Lambda^2\Pi_1\Pi_2+\alpha\frac{\partial^2}{\partial x_2^2}\Pi_1^2+\beta\frac{\partial^2}{\partial x_1^2}\Pi_2^2\Big]G,\\
w_1=&-\omega\frac{\partial^2}{\partial x_1\partial x_2}\nabla^2\Big[2c_0\Lambda^2\nabla^2-(\alpha-\beta)\Pi_1\Pi_2\Big]G,\\
w_2=&-\omega\nabla^2\Big[c_0\Lambda^2\Lambda^2\nabla^2+\alpha\frac{\partial^2}{\partial x_2^2}\Pi_1^2+\beta\frac{\partial^2}{\partial x_1^2}\Pi_2^2\Big]G,
\end{aligned}$$

$$w_3 = c_2 \frac{\partial^2}{\partial x_1 \partial x_2}\Big[(\alpha-\beta)\Lambda^2\Pi_1\Pi_2 + \alpha\frac{\partial^2}{\partial x_2^2}\Pi_1^2 + \beta\frac{\partial^2}{\partial x_1^2}\Pi_2^2\Big]G, \tag{5}$$

in which $G(x_1, x_2)$ satisfies the following twelfth-order partial differential equation:

$$\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2 G(x_1, x_2) + \nabla^2 L G(x_1, x_2) = 0, \tag{6}$$

where

$$\alpha = (\lambda+2\mu)R^2 - \omega K_1, \qquad \beta = \mu R^2 - \omega K_1, \qquad \omega = \mu(\lambda+2\mu), \tag{7a}$$

$$c_0 = \omega\frac{\mu K_2^2 + (K_1-3K_2)R^2}{\mu(K_1-K_2)-R^2}, \quad c_1 = \frac{(K_1-2K_2)R\omega}{\mu(K_1-K_2)-R^2}, \quad c_2 = \frac{(K_2\mu - R^2)\omega}{\mu(K_1-K_2)-R^2} \tag{7b}$$

$$\Pi_1 = 3\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}, \quad \Pi_2 = 3\frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_1^2}, \quad \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}, \quad \Lambda^2 = \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}, \tag{7c}$$

$$\begin{aligned} L = \frac{c_0}{\beta}\Big[&-\frac{\partial^{10}}{\partial x_1^{10}} + 5\Big(4-5\frac{\alpha}{\beta}\Big)\frac{\partial^{10}}{\partial x_1^8\partial x_2^2} - 10\Big(11-10\frac{\alpha}{\beta}\Big)\frac{\partial^{10}}{\partial x_1^6\partial x_2^4} \\ &+ 10\Big(10-11\frac{\alpha}{\beta}\Big)\frac{\partial^{10}}{\partial x_1^4\partial x_2^6} - 5\Big(5-4\frac{\alpha}{\beta}\Big)\frac{\partial^{10}}{\partial x_1^2\partial x_2^8} - \frac{\alpha}{\beta}\frac{\partial^{10}}{\partial x_2^{10}}. \end{aligned} \tag{8}$$

Assuming $R^2/(\mu K_1) \ll 1$, (this is understandable, because the coupling effect is weaker than those of phonon and phason themselves), from Eqs.(7) and (8) we obtain

$$\beta/\alpha = 1, \quad \text{and} \quad \nabla^2 L = \frac{c_0}{\beta}\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2. \tag{9}$$

Substituting Eq.(9) into Eq.(6), we find that

$$\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2\nabla^2 G(x_1, x_2) = 0, \tag{10}$$

which is the final governing equation for plane elasticity of the material.

With the aid of the generalized Hooke's law (1), the phonon and phason stress components can also be expressed in terms of G, and these expressions are omitted here due to the limitation of the space.

In other words, Eq.(5) gives a general solution in terms of G for the plane elasticity problem of an icosahedral quasicrystal. Once the function G satisfying Eq.(10) is determined for prescribed boundary conditions, the entire elastic field of an icosahedral quasicrystal can be found from Eq.(5).

3. Mode II Griffith crack problem and solutions

Consider an icosahedral quasicrystal solid with a mode II Griffith crack, which penetrates through the medium along the x_3-axis shown in Fig.1. In view of the analysis in the proceeding section, it is sufficient to study a crack of a length $2a$ occupying the interval $-a \le x_1 \le a$, $x_2 = 0$ in the x_1x_2 plane. Let a uniform shear load $\sigma_{12} = s$ in the physical space $E_\parallel$ act at infinity. For simplicity we assume that the phason stress H_{12} does not exist at infinity, i.e. $H_{12} = 0$ for $\sqrt{x_1^2+x_2^2} \to \infty$. Based on the superposition principle, the problem depicted in Fig.1 is equivalent in the sense of singularity to that shown in Fig.2, i.e. the surface of the crack is subjected to a shearing stress s and it is stress-free at the infinity. It is well-known that the singularity is a dominant factor for crack problem. By this consideration, the solution for the latter is enough, in addition, the latter is simpler than the former for mathematical treatment. We solve only the latter. Restrict our attention to the upper half-plane, owing to the symmetry of the problem considered. Then the mixed boundary conditions associated with the problem can be stated as

$$\begin{aligned} &\sigma_{12}(x_1, 0) = -s, H_{12}(x_1, 0) = 0, \quad |x_1| \le a, \\ &u_1(x_1, 0) = 0, w_1(x_1, 0) = 0, \quad |x_1| > a, \\ &\sigma_{22}(x_1, 0) = \sigma_{32}(x_1, 0) = 0, \\ &H_{22}(x_1, 0) = H_{32}(x_1, 0) = 0, \\ &-\infty < x_1 < \infty, \end{aligned} \tag{11}$$

and

$$\sigma_{ij} \to 0, \quad H_{ij} \to 0, \quad \sqrt{x_1^2+x_2^2} \to \infty\,. \tag{12}$$

To solve the mixed boundary value problem defined above, we utilize a Fourier transform

technique.[38] Upon application of the Fourier transform with respect to x_1

$$\hat{G}(\xi, x_2) = \int_{-\infty}^{\infty} G(x_1, x_2) \mathrm{e}^{-\mathrm{i}\xi x_1} \mathrm{d}x_1, \tag{13}$$

Eq.(10) can be reduced to an ordinary differential equation, of which a solution, with the infinity conditions (12) taken into account, is obtained in the following form:

$$\hat{G} = XY\mathrm{e}^{-|\xi|x_2}, \tag{14}$$

where

$$X = \Big(\frac{A_1}{\xi^8}, \frac{A_2}{|\xi^7|}, \frac{A_3}{\xi^6}, \frac{A_4}{|\xi^5|}, \frac{A_5}{\xi^4}, \frac{A_6}{|\xi^3|}\Big),$$
$$Y = (1, x_2, x_2^2, x_2^3, x_2^4, x_2^5)^{\mathrm{T}}$$

and $\hat{G}$ is the Fourier transform of G. Hence A_1, A_2, A_3, A_4, A_5 and A_6 are arbitrary functions of ξ to be determined from the boundary condition (11); the superscript T denotes the transpose operator of a matrix.

From the boundary conditions (11) and (12), we obtain the dual integral equations[38] as follows:

$$\int_0^{\infty} \xi A_j \cos\xi x_1 \mathrm{d}x_1 = s\pi b_j, \quad 0 < x_1 \le a,$$
$$\int_0^{\infty} A_j \cos\xi x_1 \mathrm{d}x_1 = 0, \quad x_1 \ge a, \tag{15}$$

in which $b_j (j = 1, 2, \ldots, 6)$ are known constants composed of elastic constants given in Appendix (A1).

The standard theory of dual integral equations provides the solution of Eq.(15) as

$$A_j = ap\pi b_j J_1(\xi a)/\xi, \tag{16}$$

where $J_1(a\xi)$ is the first-order Bessel function of the first kind.

Thus the problem is solved. By taking the Fourier inversion transform and substituting it into Eq.(5), then using the Hooke law and deformation geometry equation, the displacement and stress fields are determined. From the above results, it is easy to obtain the stress intensity factor for Mode II of the phonon field $K_{\mathrm{II}}^{\|}$—one of the most important physical quantities in fracture theory

$$K_{\mathrm{II}}^{\|} = \lim_{x_1 \to a^+} \{[2\pi(x_1 - a)]^{1/2} \sigma_{12}(x_1, 0)\} = \sqrt{\pi a} s. \tag{17}$$

The above results show that the phonon and phason stress fields, which arise from the coupling between the phonon and the phason fields, are particular for quasicrystals and exhibit a square root singularity around the crack tip. The phason stress exhibits the same singularity.

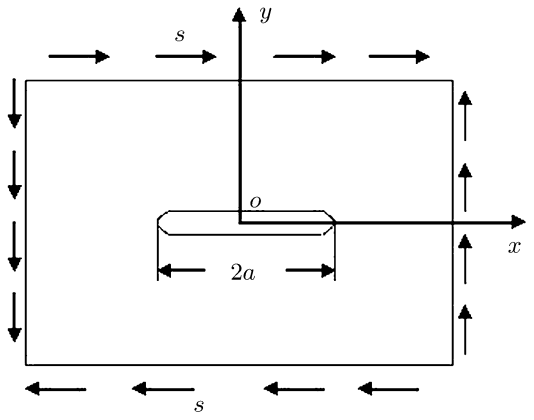


Fig.1. A mode II Griffith crack in an icosahedral quasicrystal with shearing stress at infinity.

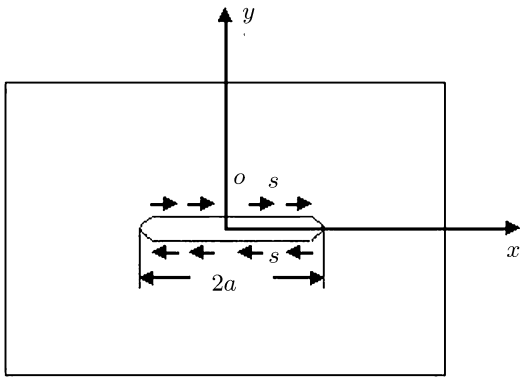


Fig.2. A mode II Griffith crack in an icosahedral quasicrystal with shearing stress at surface of the crack.

4. The crack strain energy and energy release rate

Another of the most important physical quantities in fracture theory is the crack energy release rate. The above procedure provided the total information on the displacement and stress fields for the Griffith crack. In particular, if we are concerned only with the distributions of displacement and stress along the crack line, the non-vanishing displacement and stress components are

$$u_1(x_1, 0) = \begin{cases} sM\sqrt{a^2 - x_1^2}, & |x_1| \le a, \\ 0, & |x_1| > a, \end{cases} \tag{18a}$$

$$\sigma_{12}(x_1, 0) = \begin{cases} -s, & |x_1| \le a, \\ s\Big(\dfrac{|x_1|}{\sqrt{x_1^2 - a^2}} - 1\Big), & |x_1| > a, \end{cases} \tag{18b}$$

in which M is a known constant composed of elastic constants shown in the expression (A4) of the Appendix.

Moreover, the crack strain energy W and the energy release rate $\mathcal{G}_{\rm II}$ can be respectively evaluated as

$$W_{\rm II} = \int_0^a \sigma_{12}(x_1,0)u_1(x_1,0)\mathrm{d}x_1 = M\pi a^2 s^2/2, \quad (19)$$

and

$$\mathcal{G}_{\rm II} = \frac{1}{2}\frac{\partial W}{\partial a} = M(K_{\rm II}^{\parallel})^2/2. \quad (20)$$

A comparison of the phonon displacement field, the strain energy release rate and the energy release rate with their counterparts in a conventional material indicates that they are different. These quantities reflect the contributions of phonon, phason and phonon–phason coupling, and the others coming from phonon–phason coupling. If we ignore the contributions of phason field and phonon–phason coupling, the above results reduce exactly to the well-known results in a conventional engineering material.

5. Conclusions and discussion

An icosahedral quasicrystal containing a mode II crack, which penetrates through the medium along the x_3-axis, is considered with the help of a general solution, and the analytic expressions for the displacement field and the asymptotic stress field near the crack tip are derived by Fourier transform technique. It can be seen that the stresses in phonon and phason fields around the crack tip exhibit a square root singularity and that the stress distribution is in exact agreement with the well-known results for solutions for some lower-dimensional quasicrystals given by Fan and coworkers previously. Additionally, the most important results for fracture theory: the stress intensity factor and energy release rate of the crack, have been determined analytically, which provide the basic parameters for fracture analysis for icosahedral quasicrystals.

Owing to the importance of icosahedral quasicrystal in the quasicrystalline materials, the study on its elasticity and defects is significant. The huge difficulty mathematically has been partly overcome by introducing a displacement potential,[23] we here further develop systematical the Fourier analysis and dual integral equation method to solve the mixed boundary value problem, thereby the present analytic solution for mode II Griffith crack in the material is achieved, which is significant for both fracture theory and dislocation theory, because there exists an inherent connection between dislocation and mode II crack.

Appendix Determination of constants a_j, b_j and M

In Eq.(15), $b_j (j = 1, 2, \ldots, 6)$ are

$$b_j = (-1)^{j-1}\frac{\Delta_j}{\Delta}, \quad j = 1, 2, \ldots, 6, \quad (A1)$$

where

$$\Delta = \begin{vmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{36} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{46} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{56} \\ b_{61} & b_{62} & b_{63} & b_{64} & b_{65} & b_{66} \end{vmatrix}, \quad \text{and} \quad \Delta_j = \begin{vmatrix} b_{21} & \ldots & b_{2,j-1} & b_{2,j+1} & \ldots & b_{26} \\ b_{31} & \ldots & b_{3,j-1} & b_{3,j+1} & \ldots & b_{36} \\ b_{41} & \ldots & b_{4,j-1} & b_{4,j+1} & \ldots & b_{46} \\ b_{51} & \ldots & b_{5,j-1} & b_{5,j+1} & \ldots & b_{56} \\ b_{61} & \ldots & b_{6,j-1} & b_{6,j+1} & \ldots & b_{66} \end{vmatrix}, \quad (A2)$$

in which

$$b_{11} = -2(c_2(K_1 - K_2) + c_1 R)(24\alpha - 5\beta) + RK_2(c_0(42\lambda + 45\mu) - \alpha\mu),$$

$$b_{12} = 2(c_2(K_1 - K_2) + c_1 R)(144\alpha - 49\beta) - RK_2(c_0(242\lambda + 267\mu) + 3\alpha\mu),$$

$$b_{13} = -4(c_2(K_1 - K_2) + c_1 R)(193\alpha - 98\beta) + RK_2(c_0(676\lambda + 773\mu) - 31\alpha\mu + 32\beta(\lambda + 2\mu),$$

$$b_{14} = 4(c_2(K_1 - K_2) + c_1 R)(306\alpha - 209\beta) - RK_2(c_0(1172\lambda + 1391\mu) - 129\alpha\mu + 144\beta(\lambda + 2\mu),$$

$$b_{15} = -(c_2(K_1 - K_2) + c_1 R)(1279\alpha - 1053\beta) + RK_2(c_0(675\lambda + 839\mu) - 247\alpha\mu + 288\beta(\lambda + 2\mu),$$

$$
\begin{aligned}
b_{16} &= (c_2(K_1-K_2)+c_1R)(925\alpha-821\beta)+RK_2(34c_0(31\lambda+41\mu)-265\alpha\mu+332\beta(\lambda+2\mu)\,,\\
b_{21} &= -2(c_2K_2-c_1R)(24\alpha-5\beta)+R^2(-c_0(21\lambda+2\mu)+\beta(\lambda+2\mu)-2\alpha\mu)\,,\\
b_{22} &= (c_2K_2-c_1R)(288\alpha-98\beta)+R^2(c_0(109\lambda-10\mu)-\beta(\lambda+2\mu)+14\alpha\mu)\,,\\
b_{23} &= -(c_2K_2-c_1R)(772\alpha-392\beta)-54\alpha\mu R^2-c_0(16K_1\omega+R^2(220\lambda-239\mu))\,,\\
b_{24} &= 2((c_2K_2-c_1R)(612\alpha-418\beta)-12K_1\omega(\alpha-\beta)+59\alpha\mu R^2)+5c_0(16K_1\omega+R^2(44\lambda-157\mu))\,,\\
b_{25} &= -(c_2K_2-c_1R)(1279\alpha-1053\beta)+108K_1\omega(\alpha-\beta)-145\alpha\mu R^2+c_0(-172K_1\omega-5R^2(22\lambda-216\mu))\,,\\
b_{26} &= (c_2K_2-c_1R)(925\alpha-821\beta)-198K_1\omega(\alpha-\beta)+99\alpha\mu R^2+c_0(208K_1\omega+R^2(22\lambda-1325\mu)),\\
b_{31} &= 2((c_2(K_1-K_2)+c_1R)(24\alpha-5\beta)\,,\\
b_{32} &= 2((-3(c_2(K_1-K_2)+c_1R)(32\alpha-13\beta)+16K_2\omega(\alpha-\beta))\,,\\
b_{33} &= 2((c_2(K_1-K_2)+c_1R)(170\alpha-113\beta)-72K_2\omega(\alpha-\beta))\,,\\
b_{34} &= 16c_0K_2\omega-2(c_2(K_1-K_2)+c_1R)(176\alpha-153\beta)-304K_2\omega(\alpha-\beta)\,,\\
b_{35} &= -56c_0K_2\omega+5(c_2(K_1-K_2)+c_1R)(47\alpha-43\beta)-K_2\omega(376\alpha-360\beta)\,,\\
b_{36} &= 84c_0K_2\omega-(c_2(K_1-K_2)+c_1R)(103\alpha-85\beta)+K_2\omega(288\alpha-240\beta)\,,\\
b_{41} &= 2c_0R^2(21\lambda+23\mu)\,,\\
b_{42} &= -2(16K_2\omega(\alpha-\beta)+R^2(4\alpha\mu+3c_0(37\lambda+40\mu))\,,\\
b_{43} &= 8(18K_2\omega(\alpha-\beta)+R^2(\alpha\mu+4\beta(\lambda+2\mu))+c_0(32K_2\omega+R^2(510\lambda+523\mu))\,,\\
b_{44} &= -4(64K_2\omega(\alpha-\beta)+R^2(-5\alpha\mu+28\beta(\lambda+2\mu))+c_0(112K_2\omega+25R^2(26\lambda+25\mu))\,,\\
b_{45} &= 16K_2\omega(16\alpha-15\beta)+5R^2(-9\alpha\mu+32\beta(\lambda+2\mu))+2c_0(88K_2\omega+25R^2(10\lambda+9\mu))\,,\\
b_{46} &= -K_2\omega(180\alpha-132\beta)+R^2(37\alpha\mu-116\beta(\lambda+2\mu))-2c_0(82K_2\omega+R^2(120\lambda+101\mu))\,,\\
b_{51} &= 2(c_2K_2+c_1R)(24\alpha-5\beta)-R^2(c_0(42\lambda+45\mu)-\alpha\mu)\,,\\
b_{52} &= -(c_2K_2+c_1R)(288\alpha-98\beta)+R^2(c_0(242\lambda+267\mu)-3\alpha\mu)-32\omega K_1(\alpha-\beta)\,,\\
b_{53} &= 4(c_2K_2+c_1R)(193\alpha-98\beta)+R^2(31\alpha\mu-32\beta(\lambda+2\mu))+c_0(16K_1\omega\\
&\quad -R^2(676\lambda+773\mu))-144\omega K_1(\alpha-\beta)\,,\\
b_{54} &= -(c_2K_2+c_1R)(1224\alpha-836\beta)-R^2(129\alpha\mu-144\beta(\lambda+2\mu))-c_0(64K_1\omega\\
&\quad -R^2(1172\lambda+1391\mu))-280\omega K_1(\alpha-\beta)\,,\\
b_{55} &= (c_2K_2+c_1R)(1279\alpha-1053\beta)+R^2(247\alpha\mu-288\beta(\lambda+2\mu))+2c_0(58K_1\omega\\
&\quad -R^2(375\lambda+839\mu))+\omega K_1(316\alpha-300\beta)\,,\\
b_{56} &= -(c_2K_2+c_1R)(925\alpha-821\beta)-R^2(256\alpha\mu-332\beta(\lambda+2\mu))-2c_0(62K_1\omega\\
&\quad -17R^2(31\lambda+41\mu))-\omega K_1(234\alpha-186\beta),\\
b_{61} &= 2(c_2R+c_1\mu)(24\alpha-5\beta)\,,\\
b_{62} &= 2(-(c_2R+c_1\mu)(96\alpha-39\beta)+16R\omega(\alpha-\beta))\,,\\
b_{63} &= 2((c_2R+c_1\mu)(170\alpha-113\beta)-72R\omega(\alpha-\beta))\,,\\
b_{64} &= 16c_0R\omega-(c_2R+c_1\mu)(352\alpha-306\beta)-304R\omega(\alpha-\beta)\,,\\
b_{65} &= -56c_0R\omega+5(c_2R+c_1\mu)(47\alpha-43\beta)-R\omega(376\alpha-360\beta)\,,\\
b_{66} &= 84c_0R\omega-(c_2R+c_1\mu)(103\alpha-85\beta)+R\omega(288\alpha-240\beta)\,, \qquad \text{(A3)}
\end{aligned}
$$

where α, β and ω are given by the expression (7a) in the text.

As for M in Eq.(19) in the text, it is

$$M = \sum_{j=1}^{6} a_j b_j, \tag{A4}$$

in which b_j has the same meaning as (A1), and $a_j (j = 1, 2, \ldots, 6)$ are

$$\begin{aligned}
a_1 &= -32c_0R(\lambda+\mu)\,, \quad a_2 = 16c_0R(9\lambda+11\mu)\,,\\
a_3 &= -16R(\alpha-\beta+c_0(18\lambda+25\mu))\,,\\
a_4 &= 8R(5\alpha-7\beta+c_0(42\lambda+64\mu))\,,\\
a_5 &= -10R(4\alpha-8\beta+c_0(25\lambda+41\mu))\,,\\
a_6 &= 2R(11\alpha-29\beta+c_0(60\lambda+104\mu))\,,
\end{aligned} \tag{A5}$$

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