Propagation of cracks and dislocations in 2D quasicrystals

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ABSTRACT. A closed-form solution is provided for the stress, strain and velocity fields due to a planar crack steadily propagating in an elastic quasicrystal with fivefold symmetry at speed lower than the bulk wave-speeds. The cases of a semi-infinite rectilinear crack and a Griffith crack which propagates maintaining a constant length, according to the Yoffe model, are considered. Crack face loading and remote loading conditions are taken into consideration. The dynamic theory of quasicrystal with inertia forces, but neglecting dissipative phonon activity, is assumed to govern the motion of the medium. The phonon and phason stress fields turn out to be square-root singular at crack tip. The energy release rate is positive for subsonic and subRayleigh crack propagation.

1 INTRODUCTION

Quasicrystals (QC), namely a particular class of metal alloys displaying intrinsic structure defects, attracted wide interests in the past two decades for their promising applications in many engineering fields. Their atomic structure displays symmetries forbidden by the standard classification of crystallographic groups, which are not compatible with a periodic arrangement of atoms in a cell. They indeed possess a quasi periodic structure, resulting from a continuous atomic rearrangement of the crystalline phase. In this process, the non commensurate phase, whose symmetry differs from the prevailing one, is continuously destroyed and rearranged in agreement with the prevailing atomic structure. From the point of view of mechanical modeling, the local rearrangement of atoms in a cell can be described by a phason activity, whereas the macroscopic deformation of the lattice is modeled by the phonon field as in classical elasticity. Similar structures are frequently found in aluminium alloys (Al-Cu-Fe, etc).

Dislocations play a key role as regards the mechanical properties of crystalline materials, since they influence the ductility and strength as well as the work hardening behavior. Similarly to crystals, dislocations in QCs are important for their mechanical properties. However, dislocations in QCs are special in that they are accompanied by both phonon and phason strain fields. Based on the existence of this phason strain, the characteristic features of dislocations in QC are somewhat different from those in crystals. In QC materials, the high-energy phason faults make the dislocations immobile in the low temperature range where atomic diffusion is not allowed, leading to brittle fracture occurring by an intergranular process [1,2]. QCs behave, consequently, like any intermetallic compound at room temperature and intermediate temperatures, being very brittle. However, at elevated temperatures QC materials become plastic. Dislocation motion is proposed to be one important mechanism for the high-temperature plastic deformation of Al–Cu–Fe QCs

In the present work, we investigate steady crack and dislocation propagation in an elastic QC with fivefold symmetry within the infinitesimal deformation setting, occurring at speed lower than the bulk wave velocity. A closed form solution for interactions measures, deformation, and rate fields is provided under general loading conditions. Viscous-like dissipation within material elements is neglected since the analysis is developed at a time smaller than the characteristic activation time. Stress intensity factor and energy release rate are evaluated for subsonic sub-Rayleigh crack propagation. One of the aim of the present paper is to explore the effects of phason-phonon coupling. The indeterminacy of the coupling coefficient between the gross deformation and the atomic rearrangements is accounted for parametrically. The method adopted for determining the explicit expressions of the fields investigated is an evolution of a previous approach employed in [3] for anisotropic elasticity and is based on the Stroh formalism [4]. For the considered isotropic relation between phonon stress and strain, the eigenvalue problem is degenerate, namely the fundamental matrix admits two double eigenvalues associated with a single eigenvector [5].

2 THE MODEL

The problem of a crack or dislocation propagating at constant speed v along a rectilinear path in an infinite medium is considered. A Cartesian coordinate system $(0, x, y, z)$ fixed in time and another $(0, x_1, x_2, x_3)$ moving with the defect in the x_1 direction, are considered. During steady-state propagation an arbitrary scalar or vector field $\mathbf{v}$ obeys the condition $\mathbf{v}(x_1, x_2) = \mathbf{v}(x - vt, y)$, so that $\dot{\mathbf{v}} = -v\mathbf{v}_{,1}$. By introducing the following four-dimensional vectors

$$\mathbf{t}_1 = (\sigma_{11}, \sigma_{21}, S_{11}, S_{21}), \qquad \mathbf{t}_2 = (\sigma_{12}, \sigma_{22}, S_{12}, S_{22}), \qquad \mathbf{u} = (u_1, u_2, w_1, w_2), \tag{1}$$

which collect the phonon and phason stress and displacement components, the constitutive relations for icosahedral quasicrystals introduced in [6, 7, 8] may be written in the matrix form

$$\begin{pmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \end{pmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^{\mathrm{T}} & \mathbf{C} \end{bmatrix} \begin{pmatrix} \mathbf{u}_{,1} \\ \mathbf{u}_{,2} \end{pmatrix}, \tag{2}$$

where

$$\mathbf{A} = \begin{bmatrix} 2\mu+\lambda & 0 & k_3 & 0 \\ 0 & \mu & 0 & k_3 \\ k_3 & 0 & k_1 & 0 \\ 0 & k_3 & 0 & k_1 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & \lambda & 0 & k_3 \\ \mu & 0 & -k_3 & 0 \\ 0 & -k_3 & 0 & k_2 \\ k_3 & 0 & -k_2 & 0 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \mu & 0 & -k_3 & 0 \\ 0 & 2\mu+\lambda & 0 & -k_3 \\ -k_3 & 0 & k_1 & 0 \\ 0 & -k_3 & 0 & k_1 \end{bmatrix}, \tag{3}$$

and the dynamic equilibrium equations write

$$\mathbf{t}_{1,1} + \mathbf{t}_{2,2} = \rho v^2 \mathbf{D}\, \mathbf{u}_{,11} + cv\,(\mathbf{I} - \mathbf{D})\, \mathbf{u}_{,1}, \tag{4}$$

where $\mathbf{D} = \mathrm{diag}(1, 1, 0, 0)$ and a subscript comma denotes partial differentiation with respect to spatial coordinates. The last term in (4) is due to the phason dissipation and may be neglected for sufficiently rapid propagation. Introduction of (2) in (4) yields the equations of motion in terms of the phonon and phason displacements, namely

$$\mathbf{Q}\, \mathbf{u}_{,11} + (\mathbf{B} + \mathbf{B}^{\mathrm{T}})\, \mathbf{u}_{,12} + \mathbf{C}\, \mathbf{u}_{,22} = \mathbf{0}, \tag{5}$$

where the matrix $\mathbf{Q} = \mathbf{A} - \rho v^2 \mathbf{D}$ is non singular and thus Eqn (5) may be written in the form

$$\begin{pmatrix} \mathbf{u}_{,1} \\ \mathbf{u}_{,2} \end{pmatrix}_{,1} + \begin{bmatrix} \mathbf{Q}^{-1}(\mathbf{B}+\mathbf{B}^{\mathrm{T}}) & \mathbf{Q}^{-1}\mathbf{C} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix} \begin{pmatrix} \mathbf{u}_{,1} \\ \mathbf{u}_{,2} \end{pmatrix}_{,2} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \tag{6}$$

2.1 *Degenerate eigenvalue problem*

Let us find the spectrum and corresponding eigenvectors of the 8×8 matrix of coefficients in equation (6), namely the values of ω_k, $\mathbf{e}^k$ and $\mathbf{f}^k$ satisfying the following eigenvalue problem

$$\begin{bmatrix} \mathbf{Q}^{-1}(\mathbf{B}+\mathbf{B}^{\mathrm{T}}) - \omega_k \mathbf{I} & \mathbf{Q}^{-1}\mathbf{C} \\ -\mathbf{I} & -\omega_k \mathbf{I} \end{bmatrix} \begin{pmatrix} \mathbf{e}^k \\ \mathbf{f}^k \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \tag{7}$$

The eigenvalues ω_k are the roots of the characteristic equation

$$\det[\mathbf{C} - \omega_k (\mathbf{B} + \mathbf{B}^{\mathrm{T}}) + \omega_k^2 \mathbf{Q}] = 0, \tag{8}$$

namely

$$\omega_1 = \frac{\mathrm{i}}{\sqrt{1-\dfrac{v^2}{v_1^2}}}, \qquad \omega_2 = \frac{\mathrm{i}}{\sqrt{1-\dfrac{v^2}{v_2^2}}}, \qquad \omega_3 = \omega_4 = \mathrm{i}, \tag{9}$$

as well as their corresponding conjugate pairs with negative imaginary part. In (9) we introduced the speeds of elastic wave propagation in the bulk material along the x_1 direction, namely

$$v_1 = \sqrt{\frac{2\mu + \lambda - k_3^2/k_1}{\rho}}, \qquad v_2 = \sqrt{\frac{\mu - k_3^2/k_1}{\rho}}. \tag{10}$$

For subsonic propagation the speed v is smaller than the shear wave speed v_2.

Note that the algebraic multiplicity of the root ω_3 is two, whereas the eigenvalues ω_1 and ω_2 are distinct for $v > 0$. The eigenvectors ($\mathbf{e}^k$, $\mathbf{f}^k$) corresponding to each eigenvalue ω_k , for k = 1, 2, 3, are given by the non trivial solution of the system (7). Since the eigenvalue problem (7) is degenerate, then there exists only one eigenvector for the double eigenvalue ω_3. Therefore, a generalized eigenvector ($\mathbf{e}^4$, $\mathbf{f}^4$), linearly independent of the other three, can be defined for the repeated eigenvalue ω_3 from the solution of the following linear system [4, 5]

$$\begin{bmatrix} \mathbf{Q}^{-1}(\mathbf{B}+\mathbf{B}^{\mathrm{T}}) - \omega_3 \mathbf{I} & \mathbf{Q}^{-1}\mathbf{C} \\ -\mathbf{I} & -\omega_3 \mathbf{I} \end{bmatrix} \begin{pmatrix} \mathbf{e}^4 \\ \mathbf{f}^4 \end{pmatrix} = \begin{pmatrix} \mathbf{e}^3 \\ \mathbf{f}^3 \end{pmatrix}. \tag{11}$$

Now, let us define the 4×4 matrices $\mathbf{E} = [\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3, \mathbf{e}^4]$ and $\mathbf{F} = [\mathbf{f}^1, \mathbf{f}^2, \mathbf{f}^3, \mathbf{f}^4]$ such that their columns are the eigenvectors $\mathbf{e}^k$ and $\mathbf{f}^k$, respectively, for k = 1, 2, 3, 4. Then, equations (7), for k = 1, 2, 3, and (11) can be written in the compact form

$$\begin{bmatrix} \mathbf{Q}^{-1}(\mathbf{B}+\mathbf{B}^{\mathrm{T}}) & \mathbf{Q}^{-1}\mathbf{C} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{E} & \overline{\mathbf{E}} \\ \mathbf{F} & \overline{\mathbf{F}} \end{bmatrix} = \begin{bmatrix} \mathbf{E} & \overline{\mathbf{E}} \\ \mathbf{F} & \overline{\mathbf{F}} \end{bmatrix} \begin{bmatrix} \mathbf{W}+\mathbf{N} & \mathbf{0} \\ \mathbf{0} & \overline{\mathbf{W}+\mathbf{N}} \end{bmatrix}, \tag{12}$$

where $\mathbf{W}$ and $\mathbf{N}$ are the following semisimple and nilpotent matrices

$$\mathbf{W} = \begin{bmatrix} \omega_1 & 0 & 0 & 0 \\ 0 & \omega_2 & 0 & 0 \\ 0 & 0 & \omega_3 & 0 \\ 0 & 0 & 0 & \omega_3 \end{bmatrix}, \qquad \mathbf{N} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{13}$$

respectively. Let us define the vector $\mathbf{g}(x_1, x_2)$ such that

$$\begin{pmatrix} \mathbf{u}_{,1} \\ \mathbf{u}_{,2} \end{pmatrix} = \begin{bmatrix} \mathbf{E} & \overline{\mathbf{E}} \\ \mathbf{F} & \overline{\mathbf{F}} \end{bmatrix} \begin{pmatrix} \mathbf{g} \\ \overline{\mathbf{g}} \end{pmatrix} = 2\,\mathrm{Re} \begin{pmatrix} \mathbf{E}\mathbf{g} \\ \mathbf{F}\mathbf{g} \end{pmatrix}, \tag{14}$$

then, the introduction of (14) into the differential system (6), by using the relation (12) gives

$$\mathbf{g}_{,1} + (\mathbf{W} + \mathbf{N})\, \mathbf{g}_{,2} = \mathbf{0}, \tag{15}$$

and its complex conjugate relation. The introduction of the complex variables

$$z_k = x_1 + \mathrm{i}\, x_2 \sqrt{1 - m_k^2}\,, \qquad \text{for } k = 1, 2, 3, 4, \tag{16}$$

with $m_3 = m_4 = 0$, so that $z_3 = z_4 = x_1 + \mathrm{i}\, x_2 = z$, allows writing equation (15) as

$$\frac{\partial \mathbf{g}}{\partial \bar{z}} = -\frac{\mathrm{i}}{2}\, \mathbf{N}\, \frac{\partial \mathbf{g}}{\partial z}, \qquad \Rightarrow \qquad \mathbf{g} = \mathbf{h}(z) - \frac{\mathrm{i}}{2}\, \mathbf{N} \int \frac{\partial \mathbf{g}}{\partial z}\, d\bar{z}\,. \tag{17}$$

Looking for an iterative solution, starting with $\mathbf{g} = \mathbf{h}(z)$, one may find

$$\mathbf{g}(\bar{z}, \mathbf{h}(z)) = \mathbf{h}(z) + \frac{\mathrm{i}}{2}\, \bar{z}\, \mathbf{N}\, \mathbf{h}'(z), \tag{18}$$

where the components $h_k(z_k)$, for $k = 1,2,3,4$, of vector $\mathbf{h}(z)$ are analytic functions of z_k. The corresponding displacement and stress fields, collected in the vectors $\mathbf{u}$, $\mathbf{t}_1$ and $\mathbf{t}_2$, in term of the unknown vector $\mathbf{g} = \mathbf{g}(\bar{z}, \mathbf{h}(z))$ follow from (14) and the constitutive relations (2) as

$$\mathbf{u}_{,1} = 2\,\mathrm{Re}[\mathbf{E}\,\mathbf{g}], \qquad \mathbf{u}_{,2} = 2\,\mathrm{Re}[\mathbf{F}\,\mathbf{g}], \qquad \mathbf{t}_1 = 2\,\mathrm{Re}[\mathbf{G}\,\mathbf{g}], \qquad \mathbf{t}_2 = 2\,\mathrm{Re}[\mathbf{H}\,\mathbf{g}], \tag{19}$$

where

$$\mathbf{G} = \mathbf{A}\,\mathbf{E} + \mathbf{B}\,\mathbf{F}, \qquad \mathbf{H} = \mathbf{B}^{\mathrm{T}}\,\mathbf{E} + \mathbf{C}\,\mathbf{F}. \tag{20}$$

Therefore, the stress and displacement distribution will be known once the vector $\mathbf{h}(z)$ of analytic functions has been determined for the boundary conditions of the considered problem.

3 SEMI-INFINITE CRACK LOADED ON THE CRACK SURFACES

A semi-infinite rectilinear crack steadily propagating in a quasi-crystal solid is considered. The Cartesian coordinate system $(0, x_1, x_2, x_3)$ is centered at the crack tip and moves with it. Crack surfaces are assumed to be loaded on a finite segment of length L with a uniform distribution of shear and normal phonon stresses, denoted with τ_0 and σ_0, respectively. Moreover, phonon and phason stress fields are assumed to vanish at infinity, so that the generalized stress vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ must vanish at infinity and, thus, also vectors $\mathbf{g}$ and $\mathbf{h}$.

Continuity of the phonon and phason tractions along the x_1 axis, continuity of the phonon and phason displacements along the positive x_1 axis ahead of the crack tip and the considered loading conditions on the crack surfaces require

$$\mathbf{t}_2^+(x_1, 0) = \mathbf{t}_2^-(x_1, 0), \qquad \text{for } -\infty < x_1 < \infty.$$

$$\mathbf{u}_{,1}^+(x_1, 0) = \mathbf{u}_{,1}^-(x_1, 0), \qquad \text{for } x_1 > 0. \tag{21}$$

$$\mathbf{t}_2(x_1, 0) = \begin{cases} \mathbf{q}_0 & \textit{for} \quad -L < x_1 < 0, \\ \mathbf{0} & \textit{for} \quad x_1 < -L, \end{cases}$$

respectively, where $\mathbf{q}_0 = (-\tau_0, -\sigma_0, 0, 0)$. Conditions (21) allow to define an inhomogeneous Rieman-Hilbert problem for the analytic vector function $\mathbf{g}(z, \mathbf{h}(z))$, which admits the following solution vanishing at infinity [9]:

$$\mathbf{g}(z, \mathbf{h}(z)) = \mathbf{h}(z) - \frac{\mathrm{i}}{2}\, z\, \mathbf{N}\, \mathbf{h}'(z) = \frac{1}{\pi}\, \langle\langle \frac{1}{2\mathrm{i}} \log \frac{\sqrt{z_k} + \mathrm{i}\sqrt{L}}{\sqrt{z_k} - \mathrm{i}\sqrt{L}} - \sqrt{\frac{L}{z_k}} \rangle\rangle\, \mathbf{H}^{-1}\, \mathbf{q}_0, \tag{22}$$

where $\langle\langle f_k \rangle\rangle = \mathrm{diag}(f_1, f_2, f_3, f_4)$. Since $\mathbf{N}^2 = \mathbf{0}$, then from (22) one may obtain

$$\mathbf{N}\, \mathbf{h}'(z) = \frac{1}{2\pi(z+L)} \left(\frac{L}{z}\right)^{3/2} \mathbf{N}\, \mathbf{H}^{-1}\, \mathbf{q}_0, \tag{23}$$

The introduction of (22) and (23) in (18) then yields

$$\mathbf{g}(\bar{z}, \mathbf{h}(z)) = \frac{1}{\pi}\, [\langle\langle \frac{1}{2\mathrm{i}} \log \frac{\sqrt{z_k} + \mathrm{i}\sqrt{L}}{\sqrt{z_k} - \mathrm{i}\sqrt{L}} - \sqrt{\frac{L}{z_k}} \rangle\rangle - \frac{x_2}{2\,(z+L)} \left(\frac{L}{z}\right)^{3/2} \mathbf{N}]\, \mathbf{H}^{-1}\, \mathbf{q}_0\,. \tag{24}$$

The phonon and phason displacements, collected in the vector $\mathbf{u}$ introduced in $(1)_3$, follow from direct integration of the vector $\mathbf{u}_{,1}$ in $(19)_1$ with respect to x_1, by using (24), namely

$$\mathbf{u} = \frac{2}{\pi} \mathrm{Re}\{\mathbf{E}[\langle\langle \frac{z_k+L}{2\mathrm{i}} \log \frac{\sqrt{z_k}+\mathrm{i}\sqrt{L}}{\sqrt{z_k}-\mathrm{i}\sqrt{L}} - \sqrt{L\, z_k} \rangle\rangle - x_2 \left(\frac{1}{2\mathrm{i}} \log \frac{\sqrt{z}+\mathrm{i}\sqrt{L}}{\sqrt{z}-\mathrm{i}\sqrt{L}} - \sqrt{\frac{L}{z}} \right) \mathbf{N}]\, \mathbf{H}^{-1}\}\mathbf{q}_0. \tag{25}$$

The energy release rate G for a crack propagating in a QC can be obtained by generalizing the result found for linear elastic fracture mechanics displaying square root stress singularity [10]:

$$G = -\frac{\pi}{2}\, \{ \lim_{r\to 0^+} \sqrt{r}\; \mathbf{t}_2(r)\} \cdot \{ \lim_{r\to 0^+} \sqrt{r}\; [\mathbf{u}_{,1}(r\, e^{\mathrm{i}\,\pi}) - \mathbf{u}_{,1}(r\, e^{-\mathrm{i}\,\pi})]\}. \tag{26}$$

By using $(19)_1$, $(19)_4$ and (24), the energy release rate (26) becomes

$$G = \frac{4L}{\pi}\, \mathbf{q}_0 \cdot \mathrm{Re}[\mathrm{i}\, \mathbf{E}\, \mathbf{H}^{-1}]\, \mathbf{q}_0. \tag{27}$$

Since the matrix $\mathrm{i}\, \mathbf{E}\, \mathbf{H}^{-1}$ is Hermitian, then its real part is a symmetric matrix and, thus, G turns out to be positive if $\mathrm{Re}[\mathrm{i}\, \mathbf{E}\, \mathbf{H}^{-1}]$ is positive defined.

4.1 *Free crack surface*

If the crack surfaces are traction free, then no specific load and length are present and the function $\mathbf{h}(z)$ must satisfy the homogeneous Hilbert problem defined by conditions (21) with $\mathbf{q}_0 = \mathbf{0}$. This problem admits the following solution, which vanishes at infinity [9]:

$$\mathbf{h}(z) - \frac{\mathrm{i}}{2} z\, \mathbf{N}\, \mathbf{h}'(z) = \frac{1}{2} \langle\langle \frac{1}{\sqrt{2\pi\, z_k}} \rangle\rangle\, \mathbf{H}^{-1}\, \mathbf{h}_0, \tag{28}$$

where $\mathbf{h}_0$ is a real constant vector. According to $(19)_4$ and (24), the generalized traction vector $\mathbf{t}_2$ ahead of the crack tip, at $x_2 = 0$, turns out to be $\mathbf{t}_2 = (2\,\pi\, x_1)^{-1/2}\, \mathbf{h}_0$, for $x_1 > 0$. The stress ahead of the crack tip along the x_1 axis can be written in term of the stress intensity factors for the phonon and phason stresses, collected in the vector $\mathbf{k} = (K_{II}, K_I, T_{II}, T_I)$, in the form $\mathbf{t}_2 = (2\,\pi\, x_1)^{-1/2}\, \mathbf{k}$, and thus it follows that $\mathbf{h}_0 = \mathbf{k}$. Since $\mathbf{N}^2 = \mathbf{0}$, then from (28) one obtains

$$\mathbf{N}\, \mathbf{h}'(z) = -\frac{1}{4z\sqrt{2\pi\, z}}\, \mathbf{N}\, \mathbf{H}^{-1}\, \mathbf{k}, \tag{29}$$

The introduction of (28) and (29) in (18) then yields

$$\mathbf{g}(\bar{z}, \mathbf{h}(z)) = \frac{1}{2\sqrt{2\pi}} [\langle\langle \frac{1}{\sqrt{z_k}} \rangle\rangle + \frac{x_2}{2z\sqrt{z}} \mathbf{N}]\, \mathbf{H}^{-1}\, \mathbf{k}. \tag{30}$$

The phonon and phason displacements, collected in the vector $\mathbf{u}$, can be obtained by direct integration with respect to x_1 of the vector $\mathbf{u}_{,1}$ in $(19)_1$, namely

$$\mathbf{u} = \sqrt{\frac{2}{\pi}}\, \mathrm{Re}\{\mathbf{E}\, [\langle\langle \sqrt{z_k} \rangle\rangle - \frac{x_2}{2\sqrt{z}} \mathbf{N}]\, \mathbf{H}^{-1}\, \mathbf{k}. \tag{31}$$

Moreover, from (26) by using $(19)_1$, $(19)_4$, (30) and (31) one obtains

$$G = \frac{1}{2}\, \mathbf{k} \cdot \mathrm{Re}[\mathrm{i}\, \mathbf{E}\, \mathbf{H}^{-1}]\, \mathbf{k}. \tag{32}$$

4 MOVING DISLOCATION

A steadily moving dislocation in a quasi-crystal solid is considered. The Cartesian coordinate system $(0, x_1, x_2, x_3)$ moves with it. A uniform jump in phonon and phason displacements is considered to occur along the negative x_1 axis. Continuity of phonon and phason tractions is assumed to occur therein. Moreover, phonon and phason stress fields are assumed to vanish at infinity, so that the generalized stress vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ must vanish at infinity and, thus, also vectors $\mathbf{g}$ and $\mathbf{h}$.

Continuity of the phonon and phason tractions along the x_1 axis, continuity of the phonon and phason displacements along the positive x_1 axis ahead of the crack tip and the considered jump conditions along the negative x_1 axis require

$$\begin{aligned} &\mathbf{t}_2^{+}(x_1, 0) = \mathbf{t}_2^{-}(x_1, 0), && \text{for } -\infty < x_1 < \infty. \\ &\mathbf{u}_{,1}^{+}(x_1, 0) = \mathbf{u}_{,1}^{-}(x_1, 0), && \text{for } x_1 > 0. \\ &\mathbf{u}^{+}(x_1, 0) - \mathbf{u}^{-}(x_1, 0) = \mathbf{b}, && \text{for } x_1 < 0. \end{aligned} \tag{33}$$

respectively, where **b** = (b_1, b_2, d_1, d_2) is the Burger vector collecting the gliding and climbing components of the dislocation, both for the phonon and phason fields. Conditions $(33)_{1,2}$ and the derivative of $(33)_3$ with respect to x_1 allow to define an homogeneous Riemann-Hilbert problem for the analytic function **g**(z, **h**(z)), which admits the following solution vanishing at infinity [9]:

$$\mathbf{g}(z, \mathbf{h}(z)) = \mathbf{h}(z) - \frac{\mathrm{i}}{2}\, z\, \mathbf{N}\, \mathbf{h}'(z) = \frac{1}{\pi} \langle\langle \frac{1}{z_k} \rangle\rangle\, \mathbf{q}, \tag{34}$$

where the vector **q** can be obtained as a function of **b** by using $(21)_{1,3}$. Since $\mathbf{N}^2 = \mathbf{0}$, then from (34) it follows that

$$\mathbf{N}\, \mathbf{h}'(z) = -\frac{1}{\pi} \mathbf{N} \langle\langle \frac{1}{z_k^2} \rangle\rangle\, \mathbf{q}. \tag{35}$$

The introduction of (34) and (35) in (18) then yields

$$\mathbf{g}(\bar{z}, \mathbf{h}(z)) = \frac{1}{\pi} \left(\langle\langle \frac{1}{z_k} \rangle\rangle + \frac{x_2}{z^2}\, \mathbf{N}\right) \mathbf{q}\,. \tag{36}$$

The phonon and phason displacements, collected in the vector **u** introduced in $(1)_3$, follow from direct integration of the vector $\mathbf{u}_{,1}$ in $(19)_1$ with respect to x_1, by using (36), namely

$$\mathbf{u} = \frac{2}{\pi}\, \mathrm{Re}[\mathbf{E} \left(\langle\langle \log z_k \rangle\rangle - \frac{x_2}{z} \mathbf{N}\right) \mathbf{q}]. \tag{37}$$

Finally, from (37) and $(21)_{1,3}$ one may obtain the following relations between vectors **b** and **q**

$$\mathbf{b} = 4\, \mathrm{Re}[\mathrm{i}\, \mathbf{E}\, \mathbf{q}], \qquad \mathrm{Re}[\mathrm{i}\, \mathbf{H}\, \mathbf{q}] = \mathbf{0}, \tag{38}$$

so that

$$\mathbf{q} = \frac{1}{4}\, \mathbf{H}^{-1} \{\mathrm{Re}[\mathrm{i}\, \mathbf{E}\, \mathbf{H}^{-1}]\}^{-1}\, \mathbf{b}. \tag{39}$$

5 RESULTS

Results are here reported for the constitutive coefficients in the linear constitutive relations (3) given by $\lambda = 75$ *GPa*, $\mu = 65$ *GPa*, $k_1 = 81$ *GPa*, $k_2 = -42$ *GPa* [8]. The coupling ratio $\chi = k_3/k_1$ may vary from -1 to 1. However, the mean value of k_3 is 0.1 k_1, so that $\chi = 0.1$.

The contours of phonon and phason stress components σ_{12}, σ_{22}, S_{12} and S_{22} normalized by σ_0, under Mode I loading conditions, for $\chi = 0.1$ and for the crack tip speed corresponding to $v = 0.8\, v_2$, are plotted in Fig. 1, where the coordinates are normalized by L. A significant phason stress field is induced near the crack tip as a consequence of the coupling effect provided by the constitutive equations, also for small values of the coupling parameter k_3. The corresponding phonon and phason displacement fields are plotted in Fig. 2. The distributions of the phonon stress fields are similar to the classical elastodynamic crack-tip fields [11]. In particular, for small crack tip speeds, namely for $v < 0.6\, v_2$, the opening phonon stress $\sigma_{\theta\theta}$ attains its maximum ahead of the crack tip, whereas for larger crack tip speeds the maximum opening stress occurs at about $\theta = 60°$ thus causing possible crack branching and instability. The phason stress field also exhibits the square root singularity near the crack tip, it arises from the coupling relationship between the phonon and the phason fields. The magnitude of the phason stress and displacement fields is smaller than that of the corresponding phonon fields. However, their magnitude remarkably increases for large crack tip speeds, thus denoting a corresponding increase in the phason activity.

The non-dimensional energy release rate ratio G/G_0, where G_0 is the stationary energy release rate for $v = 0$, is plotted in Fig 3 as function of the ratio v/v_2 for different values of the coupling parameter χ. Fig. 3 shows that the energy release rate G becomes unbounded as the crack tip speed approaches a limit value v_R coinciding with the Rayleigh wave speed of the material. A further increase of the crack tip speed yields a negative energy release rate ($G < 0$), so that the crack propagation turns out to be energetically not favourable at speed larger than v_R. In some cases, the energy release rate turns out to be positive at crack tip speed a bit larger than v_R, e.g. for $\chi = 0.4$ and $\chi = 0.5$. This behavior may denote an energetically favourable speed regime for speed larger than v_R, thus implying that the crack tip speed may jump of as it approaches the limit value v_R to a crack tip speed remarkably larger than v_R. The limit speed v_R varies with the coupling parameter χ according to the results plotted in Fig. 3. In particular, v_R becomes very small as χ approaches the value 0.52 from below. For $\chi > 0.52$ there exists no limit speed and crack propagation seems to be possible within the entire subsonic regime, up to the shear wave speed v_2. Note that the shear wave speed in QCs tends to vanish as the parameter χ approaches the limit value 0.89.

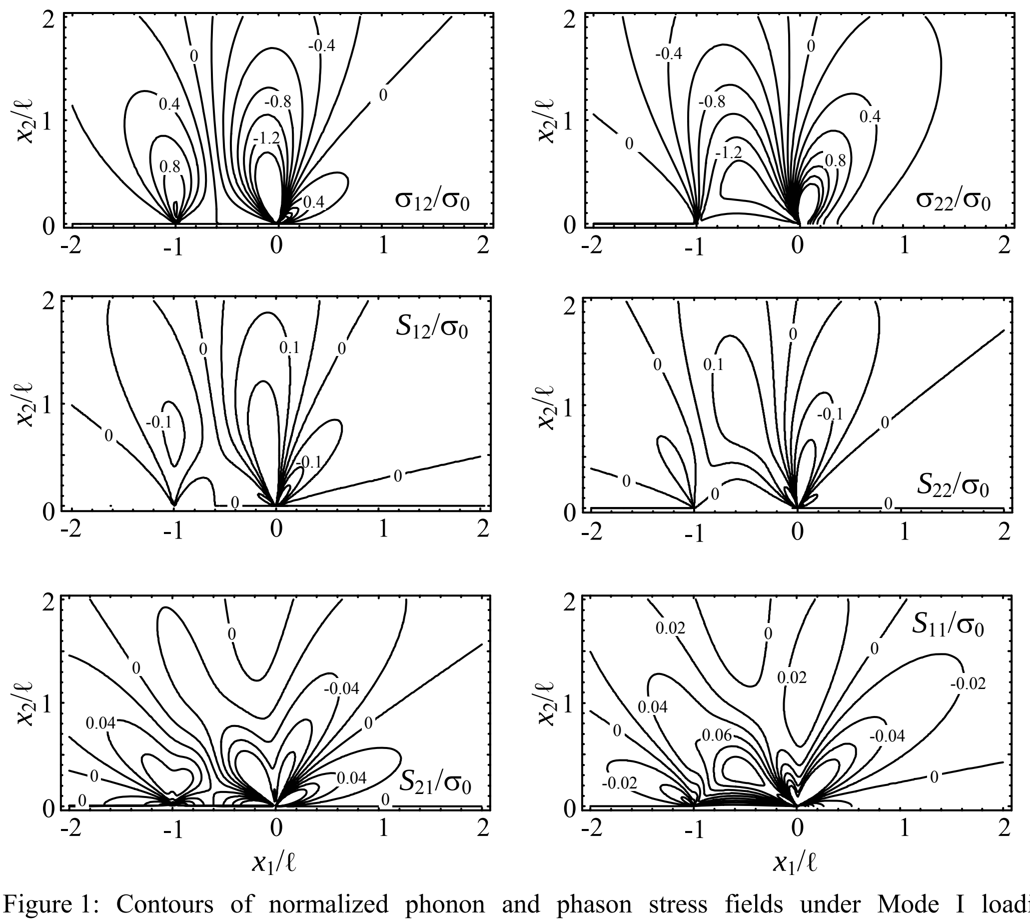

Figure 1: Contours of normalized phonon and phason stress fields under Mode I loading condition, for $\chi = 0.1$ and $v = 0.8\ v_2$.

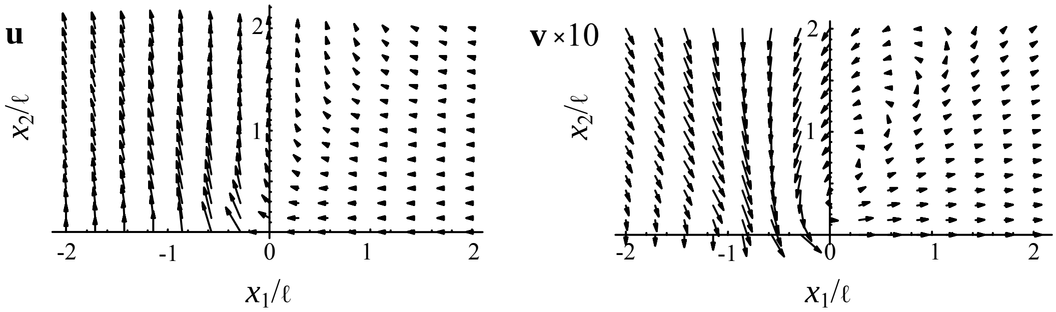

Figure 2: Phonon and phason displacement fields under Mode I loading condition, for $\chi = 0.1$ and $v = 0.8\ v_2$.

The regimes corresponding to energetically non favourable crack propagation are filled in Fig. 3. Note that as χ tends to vanish the limit crack tip speed coincides with the Rayleigh wave speed for linear elastic materials recovered for $v \approx 0.92\ v_2$.

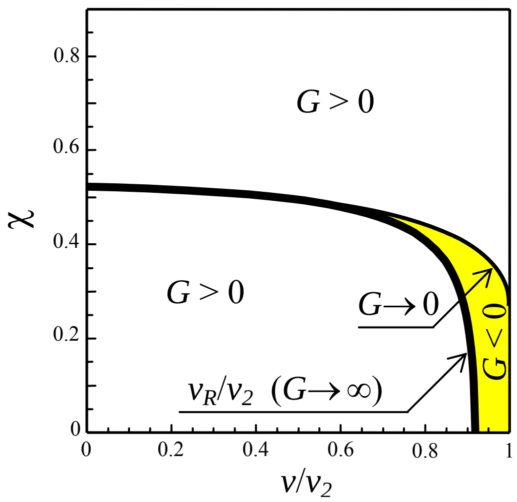

Figure 3: Energetically favourable ($G > 0$) and non-favourable ($G < 0$) regimes for crack propagation in QCs in the χ-v plane.

6 CONCLUSIONS

The results obtained for crack propagation in QC show that phonon stress fields are similar to classical elastodynamics crack-tip fields. The phason stress field displays square root singularity as the standard Cauchy stress, but its magnitude is much smaller at least for small values of the coupling parameter k_3.Phason activity increases with the parameter k_3 coupling the gross scale with the lower scale events, and also with the crack tip speed. Therefore, a significant influence of the atomic rearrangements (phason activity) is observed on the macroscopic mechanical behavior, even if the phason fields are much smaller than the phonon fields.

Moreover, the proposed method can be successfully applied to investigate a number of problems related to the presence of defects in QCs and their interactions.

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