MECHANICS OF INTERFACIAL CRACKS BETWEEN DISSIMILAR QUASICRYSTALS

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ABSTRACT

We analize the steady propagation of a straight interfacial crack between two dissimilar planar quasicrystals in pure elastic setting and infinitesimal deformation regime. A closed form solution to the balance equations is furnished. Inertia is attributed only to the macroscopic motion.

KEY WORDS: Quasicrystals, Complex bodies, Fracture

1 INTRODUCTION AND STATEMENT OF THE PROBLEM UNDER SCRUTINY

We analyze the steady propagation of a crack located at the interface between two dissimilar planar quasicrystals. The equilibrium conditions for an analogous crack between a quasi-crystalline alloy and a standard linear elastic material is also viewed in a sense as a limiting case. The formal statement of the problem under scrutiny requires preliminary notions sketched in the ensuing section.

1.1 Nature of quasicrystals

Electron diffraction experiments on $Al - Mn-$based alloys reveal the presence of atomic aggregates having point group symmetry which is inconsistent with lattice translation. The observation has been presented first in 1984 [12]. Six fivefold, ten threefold, and fifteen twofold axes characterizing icosahedral symmetry are displayed by diffraction patterns [12]. Essentially atomic clusters with pentagonal symmetry in the plane and icosahedral symmetry in the three-dimensional ambient space appear (Figure 1 furnishes a schematic picture). These symmetries are forbidden by the standard classification of crystallographic groups. A x-ray diffraction pattern obtained from the icosahedral phase could not be indexed to any Bravais lattice [12, 11, 4]. The basic reason is that the three-dimensional ambient space cannot be covered by using icosahedra only – the plane cannot be covered only by a tessellation of pentagons – a result known in elementary geometry.

To fill the space by means of icosahedra with atoms located at the vertices (alternatively the plane by means of pentagons), in fact, the insertion of topological alterations is necessary. Such alterations are due to clusters of atoms with different point group symmetry. Their formation is favoured or obstructed by the local energy landscape which can be altered by deformation induced by the interaction with the external environment.

The resulting atomic lattice is intrinsically quasi-periodic. Quasi-periodicity is determined by local rearrangements due to jumps of atoms between neighboring

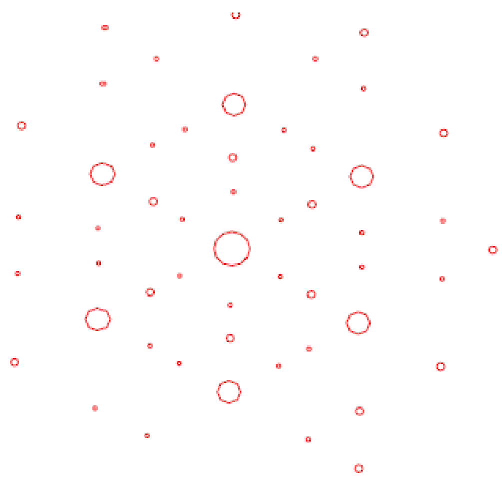

Figure 1: Cluster of atoms with icosahedral symmetry.

places and/or collective atomic modes generated for example by the flipping of crisscrossing alterations needed to maintain matching rules [2, 3, 1].

1.2 Modeling quasicrystals at continuum level

Local rearrangements of the atomic clusters do not have specific location. "Even if a quasicrystal is energetically stabilized representing a ground state, it was shown numerically that above some critical temperature the system is in a random-tiling-like phase or unlocked phase"[1].

If $\mathcal{B}$ is the region in the ambient space $\mathbb{R}^3$ occupied by a quasi-crystalline body, for example in its reference place, it is possible to assume that local atomic arrangements assuring quasi-periodicity can occur at any point x in $\mathcal{B}$. If we assume that x is representative of a sub-cluster of atoms – a material element in the common jargon of continuum mechanics – the degrees of freedom exploited in principle to generate topological alterations generating quasi-periodicity are additional to the ones associated with x itself. The latter ones are, in fact, the translational degrees of freedom of the cluster of atoms at x. Rotation of that local sub-cluster are neglected. Only local rotation between neighboring sub-clusters are accounted for. In fact, the continuum modelling implies the decision of an internal length characterizing material elements. In standard continuum mechanics such a length is not specified because degrees of freedom inside the material element are not considered. Also, here such an internal length is not specified: we define only a vector field

$$x \longmapsto \nu(x) \in \hat{\mathbb{R}}^3 \quad (1)$$

over $\mathcal{B}$, with $\hat{\mathbb{R}}^3$ a copy of the ambient space $\mathbb{R}^3$ which is distinct from it. The value $\nu(x)$ collects at each point the inner degrees of freedom exploited to assure quasi-periodicity of the atomic lattice. Commonly the field $x \longmapsto \nu(x)$ is called a **phason field** and is assumed to be differentiable. The word 'phason' recalls that it describes the potential local phase rearrangement of the atomic clusters needed for assuring quasi-periodicity (Figure 2 indicates schematically possible rearrangements).

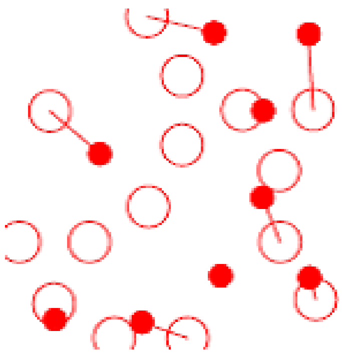

Figure 2: Sketch of rearrangements of an atomic cluster.

So, although quasi-periodicity is a global property in quasicrystals, the representation in terms of phason field [2, 3, 10, 5] constitutes an appropriate picture. In a sense, it accounts at macroscopic level for the mechanism generating quasi-periodicity rather than the periodicity itself that re-appears in the structure of the constitutive equations.

The point of view justifies the claim that the mechanics of quasicrystals in long wavelength approximation – that is the point of view of continuum mechanics – can be viewed appropriately as a special paradigmatic offspring of the general model-building of the mechanics of complex materials [7]. The adjective 'complex' is attributed to bodies characterized by a prominent influence of alterations in the material texture on the macroscopic mechanical behavior [6]. Such an influence is exerted through actions that can be hardly portrayed in terms of standard stresses. In fact, they require descriptions in terms of entities power-conjugated with the variations of appropriate geometrical descriptors of the material microstructure. In the case of quasicrystals, the descriptor of the microstructure (better of the microstructural effects) is the phason field. Non-standard actions are associated with the variation of the phason field and its gradient: they are, respectively, so-called self-actions and phason stresses. The former have purely dissipative nature and give rise to phason diffusion [10, 5]. The latter can be purely conservative [3, 2].

1.3 The problem tackled here

We consider a two-dimensional ambient space. A bi-material planar body fills the space. Precisely, a quasicrystal occupies half plane, the remaining half plane contains a quasi-crystalline alloy with different mechanical properties. The two materials are attached along a planar coherent interface.

A semi-infinite crack is located at the interface. It is indicated by $\mathcal{C}$. Figure 3 describes the situation. A frame of reference is chosen as in Figure 3. It is attached at the crack tip.

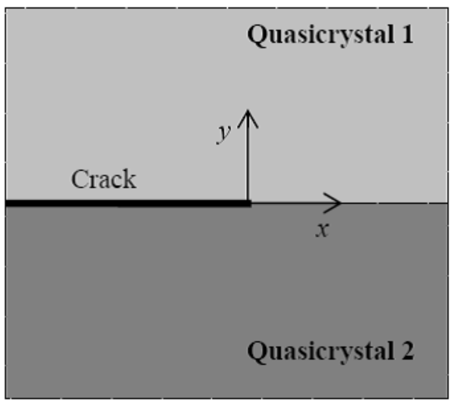

Figure 3: A bi-quasi-crystalline body with an interfacial straight crack.

In the analysis, phason diffusion in the bulk material is neglected. The attention is focused only on the purely elastic behavior in linearized setting. Dissipation can occur only at the tip of the crack when the crack opens further.

The two-dimensional setting selected here allows the use of Stroh formalism [14], a complex variable representation of balance equations in linear elasticity. We adapt it to the mechanics of quasicrystal by following the path used to describe the steady-state crack propagation of straight cracks in bodies constituted by a single type of quasicrystal [8]. When applied directly to the mechanics of quasicrystals, the procedure based on the standard Stroh formalism involves a degenerate eigenvalue problem, so appropriate modifications have to be considered [8]. The bi-material nature of the body under scrutiny here is accounted for by using an appropriate technique [13]. We furnish a closed-form solution to the balance equations for the body in Figure 3 when the margins of the cracks are not loaded and the bulk actions are neglected. Boundary conditions are prescribed at infinity and along the interface, including the crack.

2 A SUMMARY OF THE MECHANICS OF QUASICRYSTALS IN LONG WAVELENGTH APPROXIMATION

The reference place $\mathcal{B}$ is considered as a regular set in the ambient space. Macroscopic motions are described by one-to-one, orientation preserving, differentiable maps

$$(x,t) \longmapsto y := y(x,t) \in \mathbb{R}^3, \tag{2}$$

with $x \in \mathcal{B}$, $t \in [0,d]$. The displacement field u is then defined by

$$(x,t) \longmapsto u(x,t) = y(x,t) - x, \tag{3}$$

with $Du(x,t)$ its spatial derivative with respect to x. The condition $|Du| << 1$ at any x and t, characterizes the infinitesimal deformation setting.

In time, phason degrees of freedom are described by differentiable maps

$$(x,t) \longmapsto \nu(x,t) \in \hat{\mathbb{R}}^3. \tag{4}$$

Interactions associated with the rates of changes of the displacement fields are standard stresses σ (Cauchy stress tensor) and body forces b. Interactions associated with the rate of change of the microstructural phason activity are in this special case only a microstress S and a dissipative self-action ζ.

Balance equations then read as follows:

$$\operatorname{div}\sigma + b = \rho\ddot{u}, \tag{5}$$

$$\operatorname{div}\mathcal{S} = \zeta, \tag{6}$$

$$\operatorname{skw}\big(\sigma + \nu\otimes\zeta + \mathcal{S}^T N\big) = 0, \tag{7}$$

where ρ is mass density. The nature and the derivation of the balance equations from first principles has been discussed in previous works [5, 7]. Some authors claim the presence of phason inertia [2], other researchers exclude it suggesting the sole diffusive role of phason modes [10]. Here, we do not consider neither phason inertia not phason diffusion which has dissipative nature. Our analysis is restricted only to pure elastic setting.

Constitutive issues are selected in the following way:

- The stress measures σ and $\mathcal{S}$ are purely conservative. There exists an elastic energy density $e(Du, D\nu)$ such that
$$\sigma = \frac{\partial e}{\partial Du},\ \mathcal{S} = \frac{\partial e}{\partial D\nu}.$$
That e be independence of ν alone is suggested by experimental evidence [2, 3]. Independence of u is due to invariance requirements with respect to changes in observers.

- The self-action ζ is purely dissipative. So, since phason diffusion is neglected, here we assume $\zeta = 0$.

- In infinitesimal deformation setting, the elastic energy e can be considered as a quadratic form of its entries, namely
$$\begin{aligned} e(Du, D\nu) \quad = \quad & \frac{1}{2}(\mathbb{C}Du)\cdot Du + \\ & + \frac{1}{2}(\mathbb{K}D\nu)\cdot D\nu + (\mathbb{K}'D\nu)\cdot Du, \end{aligned}$$
where $\mathbb{C}$, $\mathbb{K}$ and $\mathbb{K}'$ are fourth-rank constitutive tensors. $\mathbb{C}$ is the standard elastic tensor, $\mathbb{K}'$ describes the coupling between gross deformation and phason activity, $\mathbb{K}$ is peculiar of the phason degrees of freedom. Appropriate explicit structures of the constitutive tensors are given by [2]
$$\begin{aligned} \mathbb{C}_{ijhk} &= \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \\ \mathbb{K}_{ijkl} &= k_1\delta_{ik}\delta_{jl} + k_2(\delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk}), \\ \mathbb{K}'_{ijkl} &= k_3(\delta_{i1} - \delta_{i2})(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{aligned}$$
where in the last equation no summation over repeated indices is assumed. λ and μ are the standard Lamé constants, k_1 and k_2 are associated with the pure phason activity and k_3 is the so-called *coupling coefficient*.

Once constitutive structures are substituted in the balance equations, in the two-dimensional setting treated here, the balance equations themselves can be written in matrix form by listing the components of Du and Dv in vectors. An eigenvalue problem then arises.

3 SOLUTION

In two-dimensional setting, set $\mathsf{u} := (u_1, u_2, v_1, v_2)$ and $\mathsf{t} := (\sigma_{1j}\bar{n}_j, \sigma_{2j}\bar{n}_j, \mathcal{S}_{1j}\bar{n}_j, \mathcal{S}_{2j}\bar{n}_j)$, where $\bar{n}$ is the normal to the interface. Attribute also an index $k = 1, 2$ to both u and t, with the convention that $k = 1$ refers quantities to the half-plane occupied by the first type of quasicrystal and $k = 2$ to the second one.

Solution in terms of u_k and t_k to the balance equations, under the assumptions made here, are given by

$$\mathsf{u}_{k,x} = 2\,\mathrm{Re}\left[E_k g_k\right], \quad \mathsf{t}_k = 2\,\mathrm{Re}\left[H_k g_k\right], \tag{8}$$

where no summation over repeated indices is understood from now on, and g_k can be expressed in terms of a vector function h_k as

$$g_k\left(z_k\right) = h_k\left(z_k\right) - \frac{i}{2}\bar{z}_k \mathsf{N} h_k'\left(z_k\right) \tag{9}$$

where N a nilpotent 4×4 matrix with $\mathsf{N}_{43} = 1$ and 0 in all other entries. Define

$$f_k\left(z_k\right) = h_k\left(z_k\right) - \frac{i}{2} z_k \mathsf{N} h_k'\left(z_k\right). \tag{10}$$

For $x \in \mathbb{R}$, we get $g_k\left(x\right) = f_k\left(x\right)$ and also

$$\mathsf{t}_k\left(x\right) = H_k f_k\left(x\right) + \bar{H}_k \bar{f}_k\left(x\right). \tag{11}$$

Boundary conditions along the interface read as follows:

$$\mathsf{u}_{1,x}\left(x\right) = \mathsf{u}_{2,x}\left(x\right), \quad \mathsf{t}_1\left(x\right) = \mathsf{t}_2\left(x\right), \quad x \notin \mathcal{C}, \tag{12}$$

$$\mathsf{t}_1\left(x\right) = \mathsf{t}_2\left(x\right) = 0, \quad x \in \mathcal{C}. \tag{13}$$

Moreover, it is also imposed that $g_k\left(z_k\right) \to 0$ as $\left|z_k\right| \to \infty$. The continuity of normal standard and phason stresses along the interface, namely $\mathsf{t}_1\left(x\right) = \mathsf{t}_2\left(x\right)$ for any x, yields [13] the identity $H_1 f_1\left(z\right) = \bar{H}_2 \bar{f}_2\left(z\right)$ in the half-plane with positive y, z a complex variable. As a consequence, we get

$$\bar{f}_2\left(x\right) = \bar{H}_2^{-1} H_1 f_1\left(x\right), \tag{14}$$

$$\bar{f}_1\left(x\right) = \bar{H}_1^{-1} H_2 f_2\left(x\right). \tag{15}$$

The vector $\delta\left(x\right) := \mathsf{u}_{1,x}\left(x\right) - \mathsf{u}_{2,x}\left(x\right)$ takes the form

$$\begin{aligned}\delta\left(x\right) &= E_1 f_1\left(x\right) + \bar{E}_1 \bar{f}_1\left(x\right) - \\ &\quad - E_2 f_2\left(x\right) - \bar{E}_2 \bar{f}_2\left(x\right),\end{aligned} \tag{16}$$

that is

$$\begin{aligned}\delta\left(x\right) &= \left(E_1 H_1^{-1} - \bar{E}_2 \bar{H}_2^{-1}\right) H_1 f_1\left(x\right) - \\ &\quad - \left(E_2 H_2^{-1} - \bar{E}_1 \bar{H}_1^{-1}\right) H_2 f_2\left(x\right)\end{aligned} \tag{17}$$

Define the matrix $Y_k := iE_k H_k^{-1}$ and call Z the sum

$$Z := Y_1 + \bar{Y}_2 = i\left(E_1 H_1^{-1} - \bar{E}_2 \bar{H}_2^{-1}\right). \tag{18}$$

Then, we can write

$$i\delta\left(x\right) = Z H_1 f_1\left(x\right) + \bar{Z} H_2 f_2\left(x\right). \tag{19}$$

Consider now the solution for $Z = \bar{Z}$, that is for Z a real matrix. In this case, consider

$$h\left(z\right) = \begin{cases} H_1 f_1\left(z\right), & if\ y > 0 \\ H_2 f_2\left(z\right), & if\ y < 0 \end{cases}. \tag{20}$$

The condition of vanishing standard and phason tractions at the crack margins, namely $\mathsf{t}_1\left(x\right) = \mathsf{t}_2\left(x\right) = 0$ for $x \in \mathcal{C}$, implies

$$h\left(z_k\right) = \frac{1}{2\sqrt{2\pi z_k}}\mathsf{k}, \tag{21}$$

with k a vector collecting stress intensity factors: $\mathsf{k} = \left\{K_I, K_{II}, T_I, T_{II}\right\}$, the first two entries are standard factors, the last two indicate phason factors. Moreover, in terms of k, the energy release rate $\mathcal{G}$ is given by

$$\mathcal{G} = \frac{1}{4}\mathsf{k} \cdot Z\mathsf{k}. \tag{22}$$

By taking into account that

$$f_k\left(z_k\right) = H_k^{-1} h\left(z_k\right), \tag{23}$$

then

$$h_k\left(z_k\right) = \frac{i}{2} z_k \mathsf{N} h_k'\left(z_k\right) + H_k^{-1} h\left(z_k\right), \tag{24}$$

so that

$$g_k\left(z_k\right) = H_k^{-1} h\left(z_k\right) + \frac{i}{2}\left(z_k - \bar{z}_k\right) \mathsf{N} h'\left(z_k\right), \tag{25}$$

which completes the analysis.

- The two quasicrystals occupying the plane in Figure 3 have the same Mach numbers when they have the same Lamé constants and the coupling coefficients are related by

  $$\kappa_3^{(1)} = \kappa_3^{(2)} \sqrt{\frac{\kappa_1^{(1)}}{\kappa_1^{(2)}}}. \tag{26}$$

  In this case, $z_1 = z_2$.

- The analysis of the same situation with one of the half spaces occupied by a simple linear elastic body can be considered in a sense as a limiting case by imagining to freeze the phason degrees of freedom. However, by letting to zero arbitrarily one of the two κ_3's, we realize that at least one row vanishes in a matrix that must be inverted, with the consequent difficulty. Small perturbation techniques are then necessary.

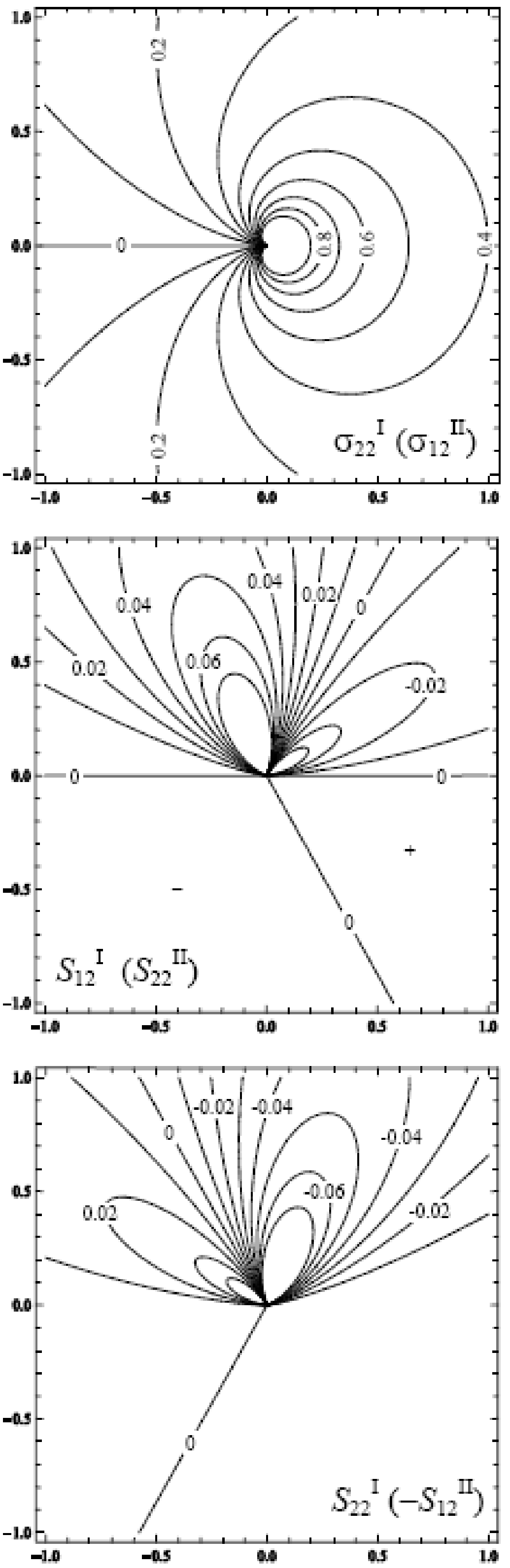

Figure 4: Contours of normalized phonon and phason stress fields for a semi-infinite rectilinear crack under remote Mode I (Mode II) loading conditions, for $\lambda^{(1)} = \lambda^{(2)} = 85GPa$, $\mu^{(1)} = \mu^{(2)} = 65GPa$, $k_1^{(1)} = k_1^{(2)} = 0.044GPa$, $k_2^{(1)} = k_2^{(2)} = 0.0396GPa$, $\chi^{(1)} = 5$ and $\chi^{(2)} = 0.1$.

Details of the analyses summarized here can be found in a forthcoming paper [9]. Figure 4 shows the portrait of the solution for the data reported in the captions, data taked from the thesis of C. Walz [15]. In the figure the crack is located in the interval $[-1, 0]$ along the horizontal axis. Figure 5 indicates sensibility of the solution interms of standard Cauchy stress with respect to the ratio

$$\chi := \frac{k_3}{k_1}, \tag{27}$$

variation due to the circumstance that the constitutive constants k_1 and k_2 can be determined with certain safety for specific classes of quasicrystals while there is a degree of uncertainty in the evaluation of the coupling coefficient k_3. The results in Figure 4 show the behaviour of the solution when phason stresses tend to vanish in one of the two quasicrystals.

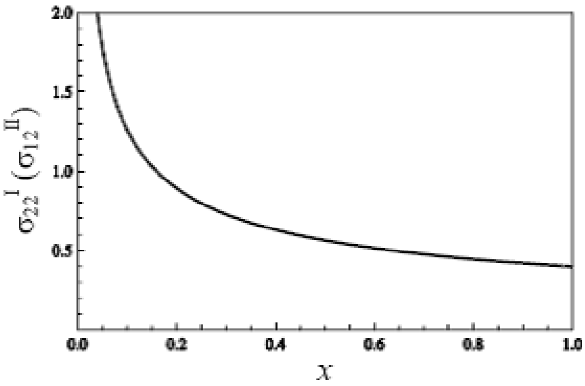

Figure 5: Variation of normalized phonon tensile (shear) stress along the interface ahead of the crack tip under remote Mode I (Mode II) loading conditions.

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