Steady-state propagation of dislocations in quasi-crystals

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We analyse the steady propagation at constant speed, lower than the shear wave-speed, of a straight dislocation in an unbounded elastic quasi-crystal with five-fold symmetry. We discuss only the ideal elastic behaviour, neglecting the dissipation associated with the atomic rearrangements. Under these conditions, we provide the expressions of phonon and phason fields in closed form. Both phonon and phason stresses appear to be singular near to the dislocation core. We also find the explicit expression of the energy per unit length around a moving dislocation.

Keywords: steady state; dislocation; quasi-crystals; Stroh formalism; phason field

1. Introduction

Quasi-crystals are inter-metallic solids characterized by long-range order and absence of the standard periodicity of crystals. Their existence has been recognized first in Shechtman et al. (1984) by evaluating diffraction patterns obtained on specimens of rapidly solidified aluminium alloys. The distribution of sharp peaks showed point group icosahedral symmetry which is incompatible with lattice translation. Such a structure is intrinsically quasi-periodic. ‘An X-ray diffraction pattern (Cu Kα source) was taken from a single-phase sample of the material containing many grains of various orientations. Had the phase consisted of a multiply twinned crystalline structure, it should have been possible to index the powder pattern regardless of the twins. The pattern obtained from the icosahedral phase could not be indexed to any Bravais lattice’ (Shechtman et al. 1984). Atomic structures with symmetry different from the prevailing one—they are called worms sometimes—produce the characteristic quasi-periodicity. They can be nucleated and annihilated in any place as a consequence of external actions. There is interplay between macroscopic deformation and local formation and/or annihilation of worms: macroscopic deformations alter the energetic content of a generic crystalline cell and may favour or obstruct local rearrangements in the atomic clusters. Atomic changes then influence the gross behaviour giving to quasi-crystal unusual electromechanical properties like low friction coefficient, high hardness, wear and oxidation resistance, high heat capacity, low heat conductivity, very large electrical resistivity, low ductility and fragile mechanical behaviour at room temperature.

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The description of quasi-crystal mechanical behaviour falls within the general framework for building models in the mechanics of complex materials: inner degrees of freedom are attributed to every material element besides the degrees of freedom in two- or three-dimensional ambient space. They are collected point by point in a vector $w$, so that a vector field—called phason field—is defined over the body. It describes rearrangements of the local atomic configuration with no change in the macroscopic shape of the body.

Quasi-periodic order admits dislocations. Their mobility influences ductility, strength and work-hardening behaviour. In contrast with crystals, not only the macroscopic displacement—called in this setting phonon field—but also the phason field can be discontinuous along a dislocation line. Burgers vector has then both phonon and phason components. In quasi-crystals, 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 (Mikulla et al. 1998; Rösch et al. 2005). Consequently, quasi-crystals display brittle behaviour at ‘room’ temperature, as it is common for intermetallic compounds. However, at elevated temperatures quasi-crystals become ductile.

Dislocation motion is crucial in high-temperature plastic deformation of Al–Cu–Fe. As a dislocation propagates, the phonon strain field relaxes instantaneously whereas the relaxation time of the phason strain is slower, as it is governed by the atomic diffusion process. At low temperature, the phason strain field requires a long time to release and it cannot move with the dislocation, thus producing a phason fault, called a phason wall, along the glide plane behind the dislocation, which inhibits further propagation and is responsible of the fragile behaviour of the material. In this situation, the elastic distortion is concentrated on the dislocation core head, whereas the phason wall extends up to its initial position and carries no distortion but only tile mismatches. At intermediate temperature, dislocations slowly migrate trailing a more or less extended phason wall. At high temperature, the atomic mobility is faster and the dislocation can migrate together with phonon and phason strains, thus increasing the capacity of dissipating mechanical energy and consequently the ductility of the material. Phonon and phason fields around a stationary dislocation have been explicitly evaluated as functions of elastic constants for several classes of quasi-crystals (e.g. Yang et al. 1995; Ricker et al. 2001). The investigation has been extended to moving dislocation in Zhu et al. (2007) by using a displacement function and in Schaaf et al. (2000) by a numerical approach.

Here, we analyse steady-state propagation of a dislocation in an elastic quasi-crystal with five-fold symmetry, and we presume that the dislocation speed be lower than the shear wave velocity. Within the multi-field description of the mechanics of quasi-crystals (see Lubensky et al. 1985; De & Pelcovits 1987; Mariano 2006), we adopt generalized elastic constitutive prescriptions (Hu et al. 2000; Ricker et al. 2001). We provide closed form expressions for phonon and phason fields for a gliding and climbing dislocation, within the infinitesimal deformation setting. We describe the influence of the coupling between the gross deformation and atomic rearrangements on the propagation of dislocations. Stroh formalism (Stroh 1958, 1962) is the tool for our analysis. However, the eigenvalue problem the analysis of balance equations leads to is degenerate, so that we are forced to modify a bit the tool that we use from its standard fashion. Technical
modification is based on what we have indicated in Radi & Mariano (2010, 2011). Finally, we also evaluate the expression of the total energy per unit length of a moving dislocation in icosahedral quasi-crystals.

2. Governing equations

We summarize here essential features of the mechanics of quasi-crystals to put in evidence what has suggested the choices made later in describing the evolution of dislocations. Here, we follow essentially what is presented earlier (Lubensky et al. 1985; De & Pelcovits 1987; Mariano 2006; foundations and general nonlinear mechanics of quasi-crystals described in the last paper).

Consider in the ambient space $\mathbb{R}^3$ an open connected set $B$ with piecewise oriented boundary. $B$ is the place occupied by a quasi-crystal in a macroscopic configuration taken as a reference. The displacement field $(x, t) \rightarrow u := u(x, t) \in \mathbb{R}^3$, $x \in B$, $t \in [0, d]$ indicates the deformed configuration at fixed instant $t$. Differentiability is assumed. The spatial derivative of $u$ at $(x, t)$ is indicated by $H$. The condition $|H| \ll 1$ defines the regime of infinitesimal strain which is the setting where our analyses develop here. In the literature on quasi-crystals, $u$ is also called a phonon field—phonons are, in fact, the particles arising in the quantization of standard elastic waves. Phonon is also used in this setting as an attribute of the common stress. We shall use at time the terminology.

At every point, the inner degrees of freedom (‘inner’ refers to the internal structure of the material element placed at the generic point $x$ in the continuum representation) exploited by the atoms in the rearrangements assuring quasi-periodicity are collected in a differentiable vector field $(x, t) \rightarrow w := w(x, t) \in \mathbb{R}^{3'}$, $x \in B$, $t \in [0, d]$, where $\mathbb{R}^{3'}$ is a copy of the ambient space $\mathbb{R}^3$ distinguished by it. As already mentioned, it is called a phason field because the atomic rearrangements imply local phase changes. The spatial derivative of $w$ is indicated by $N$.

Phonon stress, $\sigma$, and body forces, $b$, are associated in terms of power with (meaning that they develop power in) the time-rate of $u$, the phonon velocity, while another stress, $S$, called phason stress, is related with the time-rate of $w$, namely $\dot{w}$. Associated with $\dot{w}$, there is also an inner self-action. Common constitutive assumptions suggest that such an action be only of dissipative nature, so that it is equal to $c\dot{w}$, where $c$ is a positive coefficient, and is associated just with diffusion of phason models. In principle, a conservative component of the inner self-action may exist (as shown in Mariano 2006), but it is neglected in common constitutive choices presented in the available literature. Recent (not published yet) researches indicate presence of drawbacks in quasi-crystal linear elasticity that can be avoided by accounting for a conservative self-action associated with the phason field. However, the topic is not discussed further here and the common assumption is accepted. The actions just listed satisfy the following balance equations:

$$\text{div } \sigma + b = \rho \ddot{u}, \quad \text{div } S = c\dot{w} \quad \text{and} \quad \text{skw}(\sigma + w \otimes \dot{w} + S^T N) = 0, \quad (2.1)$$

where $\rho$ is the density of mass and $\dddot{u}$ the acceleration. Foundations for the two last equations for quasi-crystals can be found in Mariano (2006). Low-scale inertia for
the phason field is not foreseen in the previous balances. The existence of phason kinetic energy is controversial. The path followed in the subsequent sections could be reproduced once again in the presence of it.

The restriction to the infinitesimal deformation setting allows linear constitutive equations. In the presence of five-fold symmetry, a common choice of the constitutive relations (e.g. Hu et al. 2000) in a two-dimensional setting and with reference to a Cartesian frame \((0, x_1, x_2)\) is

\[
\begin{align*}
\sigma_{ij} &= \lambda \delta_{ij} (H_{11} + H_{22}) + \mu (H_{ij} + H_{ji}) \\
& \quad + k_3 (\delta_{i1} - \delta_{i2}) [\delta_{ij} (N_{11} + N_{22}) - N_{ij} + N_{ji}], \\
\end{align*}
\]

and

\[
\begin{align*}
S_{ij} &= k_3 [\delta_{ij} (H_{11} - H_{22}) - (\delta_{i1} - \delta_{i2}) H_{ij} + (\delta_{j1} - \delta_{j2}) H_{ji}] \\
& \quad + k_1 N_{ij} + k_2 [\delta_{ij} (N_{11} + N_{22}) - N_{ji}], \\
\end{align*}
\]

where no summation over repeated indices is understood, \(\lambda\) and \(\mu\) are standard Lamé constants, \(k_1\) and \(k_2\) are associated with the phason field and \(k_3\) is a coupling coefficient (further information on these coefficients can be found in the studies of Hu et al. (2000) and Rochal & Lorman (2002)). By using equation (2.2), balance equations (2.1) read

\[
\begin{align*}
(\lambda + 2\mu) u_{1,11} + (\lambda + \mu) u_{2,12} + \mu u_{1,22} + k_3 w_{1,11} - k_3 w_{1,22} \\
& \quad + 2k_3 w_{2,12} + b_1 = \rho \ddot{u}_1, \\
\mu u_{2,11} + (\lambda + \mu) u_{1,12} + (\lambda + 2\mu) u_{2,22} + k_3 w_{2,11} - k_3 w_{2,22} \\
& \quad + 2k_3 w_{1,12} + b_2 = \rho \ddot{u}_2, \\
k_3 u_{1,11} - k_3 u_{1,22} + 2k_3 u_{2,12} + k_1 w_{1,11} + k_1 w_{1,22} = c \ddot{w}_1 \\
\end{align*}
\]

and

\[
\begin{align*}
k_3 u_{2,11} - k_3 u_{2,22} + 2k_3 u_{1,12} + k_1 w_{2,11} + k_1 w_{2,22} = c \ddot{w}_2,
\end{align*}
\]

where the comma denotes partial differentiation. The constitutive parameter \(k_2\) does not play a role in these balances. However, the condition of positive definiteness of the strain energy density depends on the value of the parameter \(k_2\).

## 3. Steady-state propagation

We consider a dislocation propagating at constant speed \(v\) along a rectilinear path in an infinite quasi-crystalline medium. We take a Cartesian coordinate system \((0, x, y, z)\) fixed in time and another one \((0, x_1, x_2, x_3)\) moving with the dislocation in the \(x_1\) direction with speed \(v\). Steady-state propagation occurs when relevant fields, the generic one indicated by \(v\), obey the condition \(v(x_1, x_2) = v(x - vt, y)\), so that \(\dot{v} = -v \; v_1\). In a two-dimensional setting, convenience suggests the introduction of four-dimensional vectors \(t_1 = (\sigma_{11}, \sigma_{21}, S_{11}, S_{21})\) and \(t_2 = (\sigma_{12}, \sigma_{22}, S_{12}, S_{22})\), collecting phonon and phason stress components, and \(u = (u_1, u_2, w_1, w_2)\), collecting the displacement \(u\) (phonon field) and the inner degrees of freedom \(w\). The constitutive structures (2.2) recalled in §2 can be then rewritten as

\[
\begin{pmatrix}
    t_1 \\
    t_2
\end{pmatrix} =
\begin{bmatrix}
    Q & R \\
    R^T & T
\end{bmatrix}
\begin{pmatrix}
    u_1 \\
    u_2
\end{pmatrix},
\]

\(3.1\)
where
\[
Q = \begin{bmatrix}
2\mu + \lambda & 0 & k_3 & 0 \\
0 & \mu & 0 & k_3 \\
k_3 & 0 & k_1 & 0 \\
0 & k_3 & 0 & k_1 \\
\end{bmatrix}, \quad R = \begin{bmatrix}
0 & \lambda & 0 & k_3 \\
\mu & 0 & -k_3 & 0 \\
0 & -k_3 & 0 & k_2 \\
k_3 & 0 & -k_2 & 0 \\
\end{bmatrix}
\]
and
\[
T = \begin{bmatrix}
\mu & 0 & -k_3 & 0 \\
0 & 2\mu + \lambda & 0 & -k_3 \\
-k_3 & 0 & k_1 & 0 \\
0 & -k_3 & 0 & k_1 \\
\end{bmatrix}. \quad (3.2)
\]

Experiments do not allow a precise knowledge of the values to be attributed to \( k_3 \), the coefficient coupling macroscopic deformation and inner degrees of freedom. In contrast, they indicate a sort of indeterminacy. Theoretical analyses suggest upper and lower bounds for \( k_3 \). Parametric analyses in special cases help in reducing the range of \( k_3 \) variability (see Radi & Mariano 2011). The elastic energy density associated with equations (3.2) is a positive definite quadratic form in the spatial derivatives of \( u \) and \( w \), if \( \lambda + \mu > 0 \), \( k_1 > k_2 \) and \( k_3^2 < \mu(k_1 + k_2)/2 \). If the magnitude of the coupling parameter \( k_3 \) increases beyond the limit value defined by the last inequality, the strain energy density decreases and may become negative. With previous notations, the balance equations in a two-dimensional setting read
\[
t_{1,1} + t_{2,2} = \rho v^2 I_0 u_{11} + cv(I - I_0)u_{11}, \quad (3.3)
\]
where \( I \) is the identity in the space of 4 \( \times \) 4 matrices, \( I_0 = \text{diag}(1,1,0,0) \) and a subscript comma denotes partial differentiation with respect to spatial coordinates. Introduction of equation (3.1) in equation (3.3) yields
\[
\hat{Q}u_{11} + (R + R^T)u_{12} + Tu_{22} = cv(I - I_0)u_{11}, \quad (3.4)
\]
where the matrix \( \hat{Q} = Q - \rho v^2 I_0 \) is non-singular. We are interested here in analysing the evolution of a dislocation in the ideal elastic limit, obtained by letting \( c \) to zero, where equation (3.4) becomes
\[
\begin{bmatrix}
(u_1)_{,1} \\
(u_2)_{,1} \\
\end{bmatrix} + \begin{bmatrix}
\hat{Q}^{-1}(R + R^T) & \hat{Q}^{-1}T \\
-I & 0 \\
\end{bmatrix} \begin{bmatrix}
(u_1)_{,2} \\
(u_2)_{,2} \\
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
\end{bmatrix}. \quad (3.5)
\]

\((a)\) Degenerate eigenvalue problem

Eigenvalues \( \omega_k \) and eigenvectors \((e^k, f^k)\) of the 8 \( \times \) 8 matrix in equation (3.5) satisfy
\[
\begin{bmatrix}
\hat{Q}^{-1}(R + R^T) - \omega_k I \\
-I \\
\end{bmatrix} \begin{bmatrix}
\hat{Q}^{-1}T \\
-\omega_k I \\
\end{bmatrix} \begin{bmatrix}
e^k \\
f^k \\
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
\end{bmatrix}. \quad (3.6)
\]

Eigenvalues \( \omega_k \) are the roots of the characteristic equation
\[
\det[T - \omega_k(R + R^T) + \omega_k^2 \hat{Q}] = 0. \quad (3.7)
\]

They are
\[
\omega_1 = \frac{i}{\sqrt{1 - (v/v_1)^2}}, \quad \omega_2 = \frac{i}{\sqrt{1 - (v/v_2)^2}} \quad \text{and} \quad \omega_3 = \omega_4 = i, \quad (3.8)
\]
and their corresponding conjugate pairs with negative imaginary part. In equation (3.8), \( v_1 \) and \( v_2 \) are, respectively, the speeds of longitudinal and shear waves in the bulk material:

\[
v_1 = \sqrt{\frac{2\mu + \lambda - k_3^2/k_1}{\rho}} \quad \text{and} \quad v_2 = \sqrt{\frac{\mu - k_3^2/k_1}{\rho}}. \tag{3.9}
\]

For subsonic propagation, the speed \( v \) is smaller than the shear wave speed \( v_2 \). The algebraic multiplicity of the root \( u_3 \) is two, whereas the eigenvalues \( u_1 \) and \( u_2 \) are distinct for \( v > 0 \). For \( k = 1, 2, 3 \), the eigenvectors \((e^k, f^k)\) corresponding to \( u_k \) are given by the non-trivial solution of the system (3.6). Since the eigenvalue problem (3.6) is degenerate, there exists only one eigenvector for the double eigenvalue \( u_3 \).

Therefore, a generalized eigenvector \((e^4, f^4)\), which is linearly independent of the other three, can be defined for the repeated eigenvalue \( u_3 \) from the solution of the following linear system (Ting & Hwu 1998; Tanuma 2007):

\[
\begin{bmatrix}
\hat{Q}^{-1} (R + R^T) - \omega_3 I & \hat{Q}^{-1} T \\
-I & -\omega_3 I
\end{bmatrix}
\begin{bmatrix}
e^4 \\
f^4
\end{bmatrix} = \begin{bmatrix}
(w + N) 0 \\
0 W + N
\end{bmatrix}, \tag{3.10}
\]

Define \( 4 \times 4 \) matrices \( E = [e^1, e^2, e^3, e^4] \) and \( F = [f^1, f^2, f^3, f^4] \). Their columns are the generalized eigenvectors \( e^k \) and \( f^k \), respectively, for \( k = 1, 2, 3, 4 \). Equations (3.6), for \( k = 1, 2, 3 \), and equation (3.10) can be then written as

\[
\begin{bmatrix}
\hat{Q}^{-1} (R + R^T) & \hat{Q}^{-1} T \\
-I & 0
\end{bmatrix}
\begin{bmatrix}
E \\
F
\end{bmatrix} = \begin{bmatrix}
E \\
F
\end{bmatrix} \begin{bmatrix}
W + N & 0 \\
0 & W + N
\end{bmatrix}, \tag{3.11}
\]

where \( W \) and \( N \) are the following semi-simple and nilpotent matrices:

\[
W = \begin{bmatrix}
\omega_1 & 0 & 0 & 0 \\
0 & \omega_2 & 0 & 0 \\
0 & 0 & \omega_3 & 0 \\
0 & 0 & 0 & \omega_3
\end{bmatrix} \quad \text{and} \quad N = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{bmatrix}. \tag{3.12}
\]

Let \( g(x_1, x_2) \) denote a four-dimensional vector such that

\[
\begin{bmatrix}
u_1 \\
u_2
\end{bmatrix} = \begin{bmatrix}
E \\
F
\end{bmatrix} \begin{bmatrix}
g \\
f
\end{bmatrix} = 2 Re \begin{bmatrix}
Eg \\
f
\end{bmatrix}. \tag{3.13}
\]

The introduction of equation (3.13) into the differential system (3.5) and the use of the relation (3.11) give

\[
g_{,1} + (W + N)g_{,2} = 0, \tag{3.14}
\]

and its complex conjugate relation.

The introduction of the complex variables \( z_k = x_1 + i x_2 \sqrt{1 - m_k^2} \) with \( m_k = v/v_k \), for \( k = 1, 2 \), and \( z_3 = z_4 = x_1 + i x_2 = z \), allows us to reduce equation (3.14) to

\[
\frac{\partial g_k}{\partial z_k} = -\delta_{3k} \frac{i}{2} \frac{\partial g_4}{\partial z}, \quad \text{i.e.} \quad g_k = h_k(z_k) - \delta_{3k} \frac{i}{2} \frac{\partial g_4}{\partial z}, \tag{3.15}
\]

where $h_k(z_k)$, for $k = 1, 2, 3, 4$, are analytical functions of $z_k$. In compact form, equation (3.15)2 writes

$$g = h(z) - \frac{i}{2} \bar{z} h'(z), \quad (3.16)$$

where $h_k(z_k)$ is the $k$th components of the vector $h(z)$, for $k = 1, 2, 3, 4$. Corresponding strain and stress components, collected in the vectors $u_1, u_2, t_1$ and $t_2$, follow from equation (3.13) and the constitutive relations (3.1) in term of the unknown vector $g$

$$u_1 = 2 \text{Re}(E g), \; u_2 = 2 \text{Re}(F g), \; t_1 = 2 \text{Re}(G g) \; \text{and} \; t_2 = 2 \text{Re}(H g), \quad (3.17)$$

where

$$G = QE + RF \; \text{and} \; H = R^T E + TF. \quad (3.18)$$

The analytic vector $h(z)$ is determined from the specific boundary conditions selected time by time.

4. Description of the dislocation motion: closed form solution

Uniform jumps in phonon and phason fields are considered to occur along the negative $x_1$-axis, where a dislocation moves steadily, by displaying both gliding and climbing features. Continuity of phonon and phason tractions is assumed to occur therein. The generalized stress vectors $t_1$ and $t_2$ are assumed to vanish at infinity, and, thus vectors $g$ and $h$ must vanish at infinity also. Formally, the jump conditions along the $x_1$-axis require

$$t_2^+(x_1,0) - t_2^-(x_1,0) = 0, \quad \text{for} \quad -\infty < x_1 < \infty \quad (4.1)$$

and

$$u^+(x_1,0) - u^-(x_1,0) = [1 - H(x_1)] b, \quad \text{for} \quad -\infty < x_1 < \infty, \quad (4.2)$$

where $H(x_1)$ is the unit step function and $b = (b_1^\parallel, b_2^\parallel, b_1^\perp, b_2^\perp)$ is the Burger vector, which is endowed with phonon and phason components $b_1^\parallel$ and $b_1^\perp$. Both vectors $b_1^\parallel$ and $b_1^\perp$ contain gliding ($b_1^\parallel$ and $b_1^\perp$) and climbing ($b_2^\parallel$ and $b_2^\perp$) components. $b_1^\parallel$ is the phonon Burgers vector in space. $b_1^\perp$ is a Burgers vector associated with the phason vector field $w$. $b_1^\perp$ is included in the treatment for a geometrical reason: It is possible to imagine the quasi-periodic distribution of atoms constituting a quasi-crystal as generated by the projection of a periodic lattice selected in a space with dimension equal to twice the one of the ambient space over an appropriate subspace, which is identified with the physical ambient space. In this way, in the higher dimensional space it is possible to reproduce the standard (cut and paste) Volterra’s process generating dislocations. The resulting Burgers vector in the higher dimensional space has component $b_1^\parallel$ in the target subspace of the projection, while $b_1^\perp$ is the orthogonal component.

Dislocation in quasi-crystals can be classified according to the direction of the Burgers vector and strain accommodation parameter $\zeta$, defined as the ratio $\zeta = |b_1^\perp|/|b_1^\parallel|$ and thus indicating the relative amount of phonon and phason contributions. It can be represented in the form $\zeta = \tau^n$, where $\tau = (1 + \sqrt{5})/2$ is the number of the golden mean and the exponent $n$ is an integer. Experimental results obtained in Rosenfeld et al. (1995) and Feuerbacher et al. (1997a,b) show...
that the exponent \( n \) ranges between 3 and 8 for icosahedral quasi-crystals, with most frequent occurrence at \( n = 5 \). The latter value corresponds to \( \zeta = 11.1 \).

By using equation (3.17)\(_1\), it is possible to show that the continuity of phonon and phason tractions along the \( x_1 \)-axis, stated in equation (4.1), requires that the vector-valued function

\[
j(z) = \mathcal{H} \left[ h(z) - \frac{i}{2} z N h'(z) \right] - \bar{\mathcal{H}} \left[ \bar{h}(z) + \frac{i}{2} z \bar{N} \bar{h}'(z) \right]
\]

be analytic in the whole complex plane. Since \( h(z) \) must vanish at infinity, Liouville’s theorem implies that \( j(z) \) must be constant and the value of the constant must necessarily be zero. As a consequence

\[
\mathcal{H} \left[ h(z) - \frac{i}{2} z N h'(z) \right] = \bar{\mathcal{H}} \left[ \bar{h}(z) + \frac{i}{2} z \bar{N} \bar{h}'(z) \right].
\]

Derivation with respect to \( x_1 \) of equation (4.2) gives

\[
u^{+} + \nu^{-},1(x_1,0) - \nu^{-} + \nu^{-},1(x_1,0) = -d(x_1)b, \quad \text{for} \quad -\infty < x_1 < \infty.
\]

By using equation (3.17)\(_1\), the jump condition (4.5) for the phonon and phason strain at \( x_1 = 0 \) implies

\[
E \left[ h^+(x_1) - \frac{i}{2} x_1 N h^+(x_1) \right] - \bar{E} \left[ \bar{h}^+(x_1) + \frac{i}{2} x_1 \bar{N} \bar{h}^+(x_1) \right] - E \left[ h^-(x_1) - \frac{i}{2} x_1 N h^-(x_1) \right] + \bar{E} \left[ \bar{h}^-(x_1) + \frac{i}{2} x_1 \bar{N} \bar{h}^-(x_1) \right] = -\delta(x_1)b,
\]

where

\[
h^\pm(x_1) = \lim_{x_2 \to 0^\pm} h(x_1 + ix_2),
\]

so that \( \overline{h(z)}^\pm = \bar{h}^\pm(x_1) \). By assuming that the matrix \( \text{Re}(iEH^{-1}) \) be non-singular, introduction of equation (4.4) into equation (4.6) yields

\[
h^+(x_1) - \frac{i}{2} x_1 N h^+(x_1) - \left[ h^-(x_1) - \frac{i}{2} x_1 N h^-(x_1) \right] = -\frac{i}{2} \delta(x_1)H^{-1}Lb.
\]

where \( L = \left[ \text{Re}(iEH^{-1}) \right]^{-1} \). Then, Plemelj formulae imply

\[
h(z) - \frac{i}{2} z N h'(z) = \frac{1}{4\pi} \left( \frac{1}{z_k} \right) H^{-1}Lb,
\]

where the notation \( \left( \frac{1}{z_k} \right) \) denotes the diagonal matrix \( \text{diag}(f_1, f_2, f_3, f_4) \). Moreover, use of the condition \( N^2 = 0 \) in equation (4.8) yields

\[
N h'(z) = -\frac{1}{4\pi} N \left( \frac{1}{z^2_k} \right) H^{-1}Lb.
\]

Introduction of equations (4.8) and (4.9) into equation (3.16) then yields

\[
g = \frac{1}{4\pi} \left( \left( \frac{1}{z_k} \right) + \frac{x_2}{z^2} N \right) H^{-1}Lb.
\]
Once the vector $g$ is known, the vectors $t_1$ and $t_2$, collecting stress components, can be obtained from equations (3.17)_{1,2}. The vector $u$ directly follows from integration with respect to $x_1$ of equation (3.17)_{1}:

$$u = \frac{1}{2\pi} \text{Re} \left[ E \left( \langle \log z_k \rangle - \frac{x_2}{z} \right) N H^{-1} \right] Lb,$$

so that phonon and phason fields are determined.

5. Moving dislocation energy

The total energy $W$ per unit length in a cylindrical region surrounding the dislocation core and moving steadily with it is the sum of the potential energy $W_p$ and the kinetic energy $W_k$ given, respectively, by

$$W_p = \frac{1}{2} \int_A (t_1 \cdot u_{1,1} + t_2 \cdot u_{1,2}) \, dA \quad \text{and} \quad W_k = \frac{\rho v^2}{2} \int_A I_0 u_{1,1} \cdot u_{1,1} \, dA,$$

where $A$ is the annular cross section of a tube—inner radius $r_0$ and outer radius $R$—wrapped around the dislocation and extended along the $x_3$-axis. $r_0$ is the radius of the dislocation core. By using equation (3.17), we get

$$W_p = \text{Re} \int_A (Ag \cdot g + B\bar{g} \cdot g) \, dA \quad \text{and} \quad W_k = \rho v^2 \text{Re} \int_A (Cg \cdot g + D\bar{g} \cdot g) \, dA,$$

where

$$\begin{align*}
A &= G^T E + H^T F, \\
B &= G^T \bar{E} + H^T \bar{F} \\
C &= E^T I_0 E, \\
D &= E^T I_0 \bar{E}.
\end{align*}$$

Then, from equations (3.18) and (3.2) it follows that:

$$\begin{align*}
A &= E^T Q E + F^T R^T E + E^T R F + F^T T F \\
B &= E^T Q \bar{E} + F^T R^T \bar{E} + E^T R \bar{F} + F^T \bar{T} \bar{F}.
\end{align*}$$

so that matrices $A$ and $C$ are symmetric and $B$ and $D$ Hermitian, namely $B^T = \bar{B}$ and $D^T = \bar{D}$, being $Q$, $R$ and $T$ real matrices. Let us define

$$f = \frac{1}{4\pi} H^{-1} Lb,$$

and introduce a polar coordinate system $(r, \theta)$ centred at the dislocation core, with $x_1 = r \cos \theta$ and $x_2 = r \sin \theta$. From equations (4.10) and (5.5) the components of vector $g$ are $g_k = \gamma_k(\theta)/r$, where

$$\gamma_k(\theta) = \frac{f_k}{\cos \theta + i \sqrt{1 - m_k^2 \sin \theta}} + \frac{\delta_{3k} f_4 \sin \theta}{(\cos \theta + i \sin \theta)^2}.$$
Consequently, the first integral in equation (5.2) becomes

\[
W_p = \text{Re} \left[ \int_{-\pi}^{\pi} \sum_{k,j=1}^{4} (A_{kj} \gamma_k \gamma_j + B_{kj} \gamma_k \bar{\gamma}_j) \text{d}\theta \right] \ln \frac{R}{r_0} .
\]  

(5.7)

Introduction of equation (5.6) in (5.7), after integration, yields

\[
W_p = \pi \left\{ \sum_{k,j=1}^{4} \frac{4 B_{kj} f_k f_j}{\sqrt{1 - m_k^2 + \sqrt{1 - m_j^2}}} \right\} - 8 \text{Re} \left[ i f_4 \sum_{k=1}^{4} \frac{B_{3k} \bar{f}_k}{(1 + \sqrt{1 - m_k^2})^2} \right] + B_{33} \bar{f}_4 f_4 \left\{ \ln \frac{R}{r_0} \right\},
\]  

(5.8)

where \( m_3 = m_4 = 0 \). Similarly, the second integral in equations (5.2) can be evaluated as

\[
W_k = \pi \rho v^2 \left\{ \sum_{k,j=1}^{4} \frac{4 D_{kj} \bar{f}_k f_j}{\sqrt{1 - m_k^2 + \sqrt{1 - m_j^2}}} \right\} - 8 \text{Re} \left[ i f_4 \sum_{k=1}^{4} \frac{D_{3k} \bar{f}_k}{(1 + \sqrt{1 - m_k^2})^2} \right] + D_{33} \bar{f}_4 f_4 \left\{ \ln \frac{R}{r_0} \right\}.
\]  

(5.9)

The energy, as expected from the standard elastic solution (Hirth & Lothe 1982), diverges logarithmically with \( R \). The sum of equations (5.8) and (5.9) yields the total energy per unit length of the moving dislocation:

\[
W = \frac{k_p + k_k}{4\pi} \ln \frac{R}{r_0},
\]  

(5.10)

where the sum \( k_p + k_k \) indicates the pre-logarithmic energy factors.

By using equations (3.17)_4 and (3.17), the work done on the plane of the cut between \( x = r_0 \) and \( x = R \) per unit length of dislocation in a quasi-crystal becomes

\[
W_0 = -\frac{1}{2} \int_{r_0}^{R} \mathbf{t}_2(x, 0) \cdot \mathbf{b} \, \text{d}x = \frac{1}{4\pi} \mathbf{b} \cdot \mathbf{Lb} \ln \frac{R}{r_0}.
\]  

(5.11)

6. Solution in a specific case

The explicit values of the constitutive coefficients for icosahedral quasi-crystals in the linear constitutive relations (3.1) and (3.2) considered in what follows are \( \lambda = 85 \text{ GPa}, \mu = 65 \text{ GPa}, k_1 = 0.084 \text{ GPa} \) and \( k_2 = 0.036 \text{ GPa} \). They are taken from Ricker et al. (2001) and refer to an AlPdMn alloy. In that reference \( k_3 \) is considered equal to 0.408 GPa. This value corresponds to \( \chi = k_3/k_1 = 4.85 \). These constitutive parameters almost coincide with those provided in Amazit et al.
(1995) and Letoublon et al. (2001), whereas other authors suggest different values for $k_3$. A sort of experimental indeterminacy in $k_3$ is evidenced. For this reason, analyses where $k_3$ is assumed to vary parametrically in the range suggested in §3 are developed here\(^1\), limit value in the present special case being $|k_3| = 1.97$ GPa, that is, $\chi = 23.5$.

Vector plots of phonon and phason fields $u$ and $w$ are reported in figure 1 for gliding and climbing dislocation, for $\chi = 20$ and $v = 0.6 \sqrt{v_2}$. Two special situations are considered: the first one occurs for $|b|| = 1$ and $|b^\perp| = 0$—the phason component of the Burgers vector vanishes—while the other one is characterized by $|b|| = 1$ and $|b^\perp| = 11.1$. The former case simulates the presence of a phason wall behind a moving phonon dislocation—meaning that only the discontinuity of the phonon displacement field propagates, as it occurs at low temperature—the latter reproduces the simultaneous migration of both phonon and phason strains at high temperature, according to the experimental data presented in Rosenfeld et al. (1995) and Feuerbacher et al. (1997a,b) for the strain accommodation parameter $\zeta = 11.1$. The graphs of $u$ are similar for both

\(^1\)In analyzing the steady evolution of a straight crack in a planar quasi-crystal (Radi & Mariano 2011), we also performed parametric analyses, by analysing our solution sensitivity to the variation of the coupling coefficient $k_3$. The plot in fig. 9 of that paper includes $k_3$ values beyond the limit $\chi = 23.5$ for the sake of representation. Peculiar physical phenomena due to the intricate microstructural features of quasi-crystals occur below that limit.
conditions, namely with (figure 1b) and without (figure 1c) the phason wall. In the former case, however, the magnitude of the phason field near the dislocation line is very small. Conversely, in the latter situation the magnitudes of the phonon and phason fields are therein comparable.
The contours of phonon and phason stress components both for gliding and climbing dislocations in the presence of a phason wall, namely for \( \xi = 0 \), are plotted in figures 2 and 3. Similar variations have been reported in figures 4 and 5 for simultaneous migration of phonon and phason dislocation components, by assuming \( \xi = 11.1 \). The \( x_1 \) and \( x_2 \) coordinates in figures 2–5 are normalized with

Figure 6. Effects of coupling coefficient $\chi$ on phonon and phason fields, and stresses along the dislocation line for a gliding dislocation with $\mathbf{b} = (1, 0, 11.1, 0)$, for $v = 0.6\, v_2$. Solid line, $\chi = 10$; dashed line, $\chi = 20$; dotted line, $\chi = 23$. (Online version in colour.)

respect to $|\mathbf{b}|$. A fixed speed of propagation $v = 0.6\, v_2$ and two different values of the coupling parameter, namely $\chi = 10$ and $\chi = 20$, are considered therein. The distributions of the phonon stress fields are similar to that obtained in standard elasticity of simple bodies (Hirth & Lothe 1982) and display $1/r$ singularity at the dislocation core. The phason stress field is also singular near the dislocation core, even if its magnitude is much smaller than that of the phonon stress. In the presence of a phason wall, the phason stress becomes very small along the dislocation line (figures 2b, d and 3b, d), whereas for simultaneous migration of phonon and phason discontinuities the phason stress turns out to be larger therein (figures 4b, d and 5b, d). As the coupling parameter $\chi$ increases and tends to its limit value, $\chi_{\text{lim}} = 23.5$, an increment in the magnitude of the phason stress field is observed (figures 2–5b, d), accompanied however by a reduction of the phonon stress field (figures 2–5a, c).
Figure 7. Effects of the propagation speed \( v \) on phonon and phason fields, and stresses along the dislocation line for a gliding dislocation with \( \mathbf{b} = (1,0,11.1,0) \), for \( \chi = 20 \). Solid line, \( v/v_2 = 0.4 \); dashed line, \( v/v_2 = 0.6 \); dotted line, \( v/v_2 = 0.8 \). (Online version in colour.)

The coupling of phonon and phason fields along the dislocation line \( x_2 = 0 \) is also depicted in figure 6 for a gliding dislocation. As the coupling parameter \( \chi \) increases, \( u_2 \) and \( w_2 \) reduce in amplitude, so is for the phonon stress, whereas no remarkable changes in the phason stress are observed along the dislocation line. In contrast with this result, for a stationary dislocation in an icosahedral quasi-crystal, different from that considered here, results in Zhu et al. (2007) show that the phonon field increases with the growth of the coupling parameter. As expected for the considered value of the strain accommodation parameter \( \zeta = 11.1 \), the phason field along the dislocation line is larger than the phonon displacement.

The effect of the propagation speed on the variations of phonon and phason fields is illustrated in figure 7 for a gliding dislocation. As the propagation of the dislocation becomes faster, an increase in the displacement \( u_2 \) and phason field \( w_2 \) along the dislocation line is observed, whereas the phonon and phason stress fields
are scarcely affected by the value of the propagation speed. Effects of coupling parameter and propagation speed similar to those observed in figures 6 and 7 for a gliding dislocation have been observed also for a climbing dislocation.

The variations of the total energy $W$, potential energy $W_p$ and kinetic energy $W_k$ (per unit length) are plotted in figure 8 as functions of the ratio $v/v_2$ for two different values of the coupling parameter $\chi$. For a gliding dislocation, the
energy per unit length becomes unbounded as the propagation speed approaches the limit value $v_2$ coinciding with the shear wave speed of the quasi-crystal (figure 8a,b). When $\chi$ increases from 10 to 20, a remarkable reduction of the total energy per unit length appears. This behaviour is expected since the strain energy density decreases and may become negative when the magnitude of the coupling parameter $\chi$ increases and exceeds the limit value $\chi = 23.5$ defined in §3 and corresponding to the loss of positive definiteness of the strain energy density. This effect clearly shows in quasi-crystals the influence of the low-scale effects on the macroscopic behaviour.

At low propagation speed the energy around a gliding dislocation is slightly lower than around a climbing dislocation (figure 9). Conversely, at fast speed the energy around a gliding dislocation becomes much larger than around a climbing dislocation. These analytical results are in good agreement with the experimental observations presented in Mompiou et al. (2003, 2004), where glide dislocations are found to propagate much slower than climbing dislocations.

7. Remarks

The restriction of our analyses to the linear elastic case suggests to attribute an ideal limit character to our results. In fact, microstructural dissipation may play a non-negligible role. Also, in principle, it is possible to foresee the presence of a conservative self-action (as derived in Mariano (2006)), a self-action commonly neglected a priori (as already mentioned). Relevant analyses present additional difficulties.

In any case, the restricted setting we have worked in allows us to underline analogies and differences with the analysis of steadily moving dislocations in simple linear elastic materials. Micro-to-macro interaction appears in the following aspects:

— the magnitudes of phonon and phason fields are proportional to the speed of propagation;
— as the phason–phonon coupling coefficient increases, the magnitudes of phonon and phason fields, and phonon stress decrease, whereas the amplitude of the phason stress increases;
— the coupling between phonon and phason fields produces a remarkable reduction of the total energy per unit length around a propagating dislocation, together with a reduction of the amplitude of displacement and phason field; and
— at low speed, gliding dislocations require for their propagation an energy amount lower than climbing dislocations, whereas at high speed an opposite trend is observed.

E.R. gratefully acknowledges financial support from ‘Cassa di Risparmio di Modena’ within the framework of the International Research Project 2009–2010 ‘Modelling of crack propagation in complex materials’. The work by P.M.M has been developed within the programmes of the research group in ‘Theoretical Mechanics’ of the ‘Centro di Ricerca Matematica Ennio De Giorgi’ of the Scuola Normale Superiore at Pisa. He also acknowledges the support of GNFM-INDAM.
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