

Elastic theory of icosahedral quasicrystals – application to straight dislocations

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Abstract. In quasicrystals, there are not only conventional, but also phason displacement fields and associated Burgers vectors. We have calculated approximate solutions for the elastic fields induced by two-, three- and fivefold straight screw- and edge-dislocations in infinite icosahedral quasicrystals by means of a generalized perturbation method. Starting from the solution for elastic isotropy in phonon and phason spaces, corrections of higher order reflect the two-, three- and fivefold symmetry of the elastic fields surrounding screw dislocations. The fields of special edge dislocations display characteristic symmetries also, which can be seen from the contributions of all orders.

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1 Introduction

It has been demonstrated frequently (see, *e.g.*, [1]) that in quasicrystals, as in periodic crystals, plasticity is caused by dislocations moving under external stresses. If the elastic fields around dislocations are known, their influence on the lattice and the interaction between dislocations can be calculated. In quasicrystals, dislocations are surrounded not only by phononic, but also by phasonic elastic fields. They are described by a generalization of the standard elastic equations. The generalized elastic theory has become a powerful and important tool for studying the mechanical behaviour of quasicrystals.

The dislocation problem is solved when the medium's elastic Green's function is available. The elastic Green's function has been established in closed form for isotropic [2] and hexagonal [3] ordinary media, and for pentagonal [4], decagonal and dodecagonal [5] quasicrystals. An approximate solution for the elastic Green's function of icosahedral quasicrystals is given in [6]. In this paper, the results are obtained by direct solution of the equations of balance instead by use of Green's method.

Analytical solutions for the elastic fields around dislocations exist only for the above mentioned cases [2–5]. In this paper, we present the solution for icosahedral quasicrystals in terms of appropriate perturbation series.

The structure of the paper is as following. Starting from the density wave picture, we summarize in Section 2 the generalized elastic theory of icosahedral quasicrystals, including dislocation elastic theory. Section 3 deals with the generalized projection method as one possibility to

solve the dislocation problem. Here we present a set of recursion formulae, which can be used to calculate perturbation expansions of the elastic fields. In the last section, we discuss displacement fields induced by different types of fivefold dislocations in icosahedral quasicrystals.

Most concepts and notations in this paper are identical to those used in [6].

2 Elastic theory of icosahedral quasicrystals

2.1 Some fundamentals

A quasicrystal is a translationally ordered structure with sharp diffraction pattern exhibiting non-crystallographic symmetry. For this reason, its mass density $\rho(\mathbf{x})$ can be written as a sum over density waves:

$$\rho(\mathbf{x}) = \sum_{\mathbf{k} \in L} \rho_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}} = \sum_{\mathbf{k} \in L} |\rho_{\mathbf{k}}| e^{i(\mathbf{k} \cdot \mathbf{x} + \phi_{\mathbf{k}})}. \quad (1)$$

Here, L is a module over the reciprocal quasilattice. The numbers $\phi_{\mathbf{k}}$ are the phases of the complex coefficients $\rho_{\mathbf{k}}$.

For icosahedral quasicrystals, the diffraction pattern and L display icosahedral point symmetry. Six vectors \mathbf{k}_{α} , $\alpha = 1, \dots, 6$, pointing to appropriate six of the vertices of an icosahedron can serve as a basis of L . Phenomenological Landau theory [7, 8] shows that there are six degrees of freedom, which can be interpreted as the phases $\phi_{\mathbf{k}_{\alpha}}$ of the basis vectors. Thus, a frequently used approach is the extension of the density (1) to the density of a periodic structure in six-dimensional hyperspace, which can be subjected to a six-dimensional displacement field γ .

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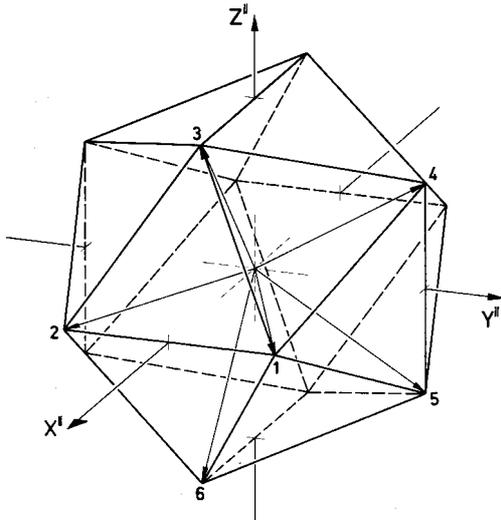


Fig. 1. The projections $\mathbf{P}^{\parallel} \mathbf{e}_{\alpha}$ of the six natural hyperspace basis vectors \mathbf{e}_{α} onto E^{\parallel} . From [9].

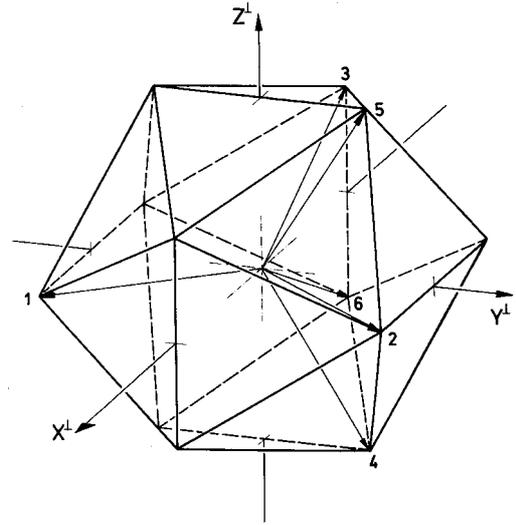


Fig. 2. The projections $\mathbf{P}^{\perp} \mathbf{e}_{\alpha}$ of the six natural hyperspace basis vectors \mathbf{e}_{α} onto E^{\perp} . From [9].

(1) is recovered by a cut of the hyperperiodic structure by physical space [9]. A parametrization of the $\phi_{\mathbf{k}}$ is

$$\phi_{\mathbf{k}} = \phi_{\mathbf{k},0} - \boldsymbol{\kappa} \cdot \boldsymbol{\gamma}, \quad (2)$$

which involves vectors $\boldsymbol{\kappa}$ belonging to the reciprocal hyperlattice in six dimensions. The set $\{\boldsymbol{\kappa}_{\alpha}\}$ must be linearly independent over the real numbers and serves as basis of the reciprocal hyperlattice, which is usually chosen to be hypercubic. Then, the direct hyperlattice is hypercubic also, with basis vectors $\boldsymbol{\varrho}_{\beta}$, $\beta = 1, \dots, 6$, defined by [7]

$$\boldsymbol{\kappa}_{\alpha} \cdot \boldsymbol{\varrho}_{\beta} = 2\pi \delta_{\alpha\beta}. \quad (3)$$

The icosahedral group Y acts on the hyperspace according to the reducible six-dimensional representation $\Gamma^6 = \Gamma^3 \oplus \Gamma^{3'}$. The hyperspace decomposes into two orthogonal, three-dimensional invariant subspaces E^{\parallel} and E^{\perp} , belonging to the irreducible representations Γ^3 (vector representation) and $\Gamma^{3'}$ of Y . E^{\parallel} is the physical or parallel space and E^{\perp} the perpendicular space. Two projection operators \mathbf{P}^{\parallel} and \mathbf{P}^{\perp} can be applied to hyperspace vectors to obtain their respective components in E^{\parallel} and E^{\perp} . This procedure is shown in Figures 1, 2 for the ortho-normal natural basis $\{\mathbf{e}_{\alpha}\}$, spanning a hypercube in six-dimensional hyperspace.

All quantities depend on the physical space coordinates $\mathbf{x}^{\parallel} = \mathbf{x}$ only. Because of the orthogonality of E^{\parallel} and E^{\perp} , equation (2) can be written

$$\phi_{\mathbf{k}} = \phi_{\mathbf{k},0} - \mathbf{k}^{\parallel} \cdot \mathbf{u} - \mathbf{k}^{\perp} \cdot \mathbf{w}. \quad (4)$$

Notations $\boldsymbol{\kappa} = \mathbf{k}^{\parallel} \oplus \mathbf{k}^{\perp}$ and $\boldsymbol{\gamma} = \boldsymbol{\gamma}^{\parallel} \oplus \boldsymbol{\gamma}^{\perp} = \mathbf{u} \oplus \mathbf{w}$ are used, where $\mathbf{k}^{\parallel} = \mathbf{k} \in L$. \mathbf{u} is the ordinary phonon displacement, whose character is propagating. \mathbf{w} is the phasonic displacement with diffusive character [10]. In the atomic picture, non-vanishing \mathbf{w} -fields lead to local rearrangements of atoms, which are called phasonic flips.

Spatially varying $\boldsymbol{\gamma}$ and $\phi_{\mathbf{k}}$, respectively, belong to deformed states, which can be described by the elastic tensor fields of distortion $\boldsymbol{\beta}$ and strain $\boldsymbol{\varepsilon}$ defined by

$$\mathbf{d}\mathbf{u} = \boldsymbol{\beta}^u \mathbf{d}\mathbf{x}, \quad \mathbf{d}\mathbf{w} = \boldsymbol{\beta}^w \mathbf{d}\mathbf{x}, \quad \boldsymbol{\beta} = \begin{bmatrix} \boldsymbol{\beta}^u \\ \boldsymbol{\beta}^w \end{bmatrix}, \quad (5)$$

$$\boldsymbol{\varepsilon}^u = \frac{1}{2} (\boldsymbol{\beta}^u + \boldsymbol{\beta}^{u,t}), \quad \boldsymbol{\varepsilon}^w = \boldsymbol{\beta}^w, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \boldsymbol{\varepsilon}^u \\ \boldsymbol{\varepsilon}^w \end{bmatrix}. \quad (6)$$

In case of single-valued displacement fields \mathbf{u} and \mathbf{w} ,

$$\beta_{ij}^u = \frac{\partial u_i}{\partial x_j}, \quad \beta_{ij}^w = \frac{\partial w_i}{\partial x_j}, \quad (7)$$

$$\varepsilon_{ij}^u = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad \varepsilon_{ij}^w = \frac{\partial w_i}{\partial x_j}, \quad (8)$$

where $i, j \in \{1, 2, 3\}$. The six symmetric and three anti-symmetric components of $\boldsymbol{\beta}^w$ mix under the action of Y , and therefore no invariants can be constructed from the symmetric or antisymmetric components of $\boldsymbol{\beta}^w$ only. So due to (6), the phason strain tensor $\boldsymbol{\varepsilon}^w$ must be the full $\boldsymbol{\beta}^w$ to contribute to the elastic energy density F .

The relations (6) and (8) hold in the linear regime $|\frac{\partial u_i}{\partial x_j}|, |\frac{\partial w_i}{\partial x_j}| \ll 1$, which we are interested in. Linear elasticity is described by an elastic energy density which is an Y -invariant quadratic form of the components of $\boldsymbol{\varepsilon}$:

$$F = \frac{1}{2} C_{\alpha i \beta j} \varepsilon_{\alpha i} \varepsilon_{\beta j} = \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{C} \boldsymbol{\varepsilon}. \quad (9)$$

Here, the Greek indices $\alpha, \beta \in \{1, \dots, 6\}$ refer to E^{\parallel} ($\alpha, \beta \in \{1, 2, 3\}$) and to E^{\perp} ($\alpha, \beta \in \{4, 5, 6\}$). This is different from the meaning of α, β in equation (3).

Differentiation of (9) leads to the generalized Hooke's law:

$$\sigma_{\alpha i} = \frac{\partial F}{\partial \varepsilon_{\alpha i}} = C_{\alpha i \beta j} \varepsilon_{\beta j}, \quad \boldsymbol{\sigma} = \mathbf{C} \boldsymbol{\varepsilon}, \quad (10)$$

with the generalized stress field

$$\boldsymbol{\sigma} = \begin{bmatrix} \boldsymbol{\sigma}^u \\ \boldsymbol{\sigma}^w \end{bmatrix}, \quad (11)$$

where $\boldsymbol{\sigma}^u = \boldsymbol{\sigma}^{u,t}$ is symmetric. The stress tensors $\boldsymbol{\sigma}^{u,w}$, applied to normal vectors \mathbf{n} of real or fictitious surfaces in physical space, lead to surface forces $\mathbf{t}^{u,w} = \boldsymbol{\sigma}^{u,w} \mathbf{n}$, which must be applied to keep the system in balance. These forces have components in E^{\parallel} and E^{\perp} , respectively, and are combined to $\mathbf{t} = \mathbf{t}^u \oplus \mathbf{t}^w$ [11]. Besides the conventional body force \mathbf{f}^u , an analogous force \mathbf{f}^w with direction in E^{\perp} has to be introduced to formulate the generalized equations of balance consistently. We use the notation $\mathbf{f} = \mathbf{f}^u \oplus \mathbf{f}^w$.

Hooke's law can be formulated very simply with the help of group theory. Due to equations (6), $\boldsymbol{\varepsilon}^u$ transforms as the representation $(\Gamma^3 \otimes \Gamma^3)_{\text{sym}} = \Gamma^1 \oplus \Gamma^5$ under actions of Y, whereas $\boldsymbol{\varepsilon}^w$ transforms as $\Gamma^3 \otimes \Gamma^{3'} = \Gamma^4 \oplus \Gamma^5$. The transformations of the components of $\boldsymbol{\sigma}^{u,w}$ are quite the same. With the irreducible strain components related to the coordinate systems of Figures 1 and 2,

$$\boldsymbol{\varepsilon}_1^u = [\varepsilon_{\Gamma^1}^u]^t = [\varepsilon_{\Gamma^1}^u], \quad \boldsymbol{\varepsilon}_5^u = [\varepsilon_{\Gamma^5}^u, \dots, \varepsilon_{\Gamma^5}^u]^t, \quad (12)$$

$$\boldsymbol{\varepsilon}_4^w = [\varepsilon_{\Gamma^4}^w, \dots, \varepsilon_{\Gamma^4}^w]^t, \quad \boldsymbol{\varepsilon}_5^w = [\varepsilon_{\Gamma^5}^w, \dots, \varepsilon_{\Gamma^5}^w]^t,$$

(see [12] and Appendix A) and analogous vectors containing the irreducible stresses, Hooke's law reads

$$\begin{bmatrix} \boldsymbol{\sigma}_1^u \\ \boldsymbol{\sigma}_5^u \\ \boldsymbol{\sigma}_4^w \\ \boldsymbol{\sigma}_5^w \end{bmatrix} = \begin{bmatrix} \mu_1 & 0 & 0 & 0 \\ 0 & \mu_2 & 0 & \mu_3 \\ 0 & 0 & \mu_4 & 0 \\ 0 & \mu_3 & 0 & \mu_5 \end{bmatrix} \begin{bmatrix} \boldsymbol{\varepsilon}_1^u \\ \boldsymbol{\varepsilon}_5^u \\ \boldsymbol{\varepsilon}_4^w \\ \boldsymbol{\varepsilon}_5^w \end{bmatrix}. \quad (13)$$

Since only equal-indexed components of the same irreducible representation can interact with each other, the number of independent second-order elastic constants is restricted to five. The elastic energy density corresponding to (13) is

$$F = \frac{1}{2} \mu_1 \boldsymbol{\varepsilon}_1^u \cdot \boldsymbol{\varepsilon}_1^u + \frac{1}{2} \mu_2 \boldsymbol{\varepsilon}_5^u \cdot \boldsymbol{\varepsilon}_5^u + \mu_3 \boldsymbol{\varepsilon}_5^u \cdot \boldsymbol{\varepsilon}_5^w + \frac{1}{2} \mu_4 \boldsymbol{\varepsilon}_4^w \cdot \boldsymbol{\varepsilon}_4^w + \frac{1}{2} \mu_5 \boldsymbol{\varepsilon}_5^w \cdot \boldsymbol{\varepsilon}_5^w. \quad (14)$$

A comparison with (9) yields the coefficients $C_{\alpha i \beta j}$. In Appendix C, we discuss the conventions for independent elastic constants used by other authors.

Mechanical stability requires $F > 0$ for every $\boldsymbol{\varepsilon} \neq 0$, which is fulfilled when all eigenvalues of the elastic tensor of (13) are positive. This leads to the following constraints on the elastic constants: $\mu_1 > 0$, $\mu_2 > 0$, $\mu_4 > 0$, $\mu_5 > 0$, and $\mu_2 \mu_5 > \mu_3^2$.

According to (13) and (14), the elastic constants μ_1 and μ_2 describe pure phonon elasticity. Without phason elasticity, for example on a short time scale, icosahedral quasicrystals behave like isotropic media with the two Lamé-constants

$$\lambda = \frac{1}{3}(\mu_1 - \mu_2), \quad \mu = \frac{1}{2} \mu_2. \quad (15)$$

They can be measured by ultrasound transmission [13]. The elastic constants μ_4 and μ_5 belong to pure phason elasticity. They are determined currently only indirectly from diffuse scattering around Bragg peaks [14]. Values for the phason-phason-coupling μ_3 have been calculated in computer simulations to have much smaller absolute values than the two phononic elastic constants [15].

Isotropic phonon elasticity in thermal equilibrium requires decoupled phonon and phason elasticity, *i.e.* $\mu_3 = 0$. Isotropy in phason elasticity is given in the spherical approximation $\mu_4 = \mu_5$ discussed in [6], in addition to the condition $\mu_3 = 0$.

Gauss' theorem, applied to equation (10), provides the well-known elastic equations of balance in generalized form:

$$\text{div } \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0}, \quad \frac{\partial}{\partial x_i} \sigma_{\alpha i} + f_{\alpha} = 0, \quad (16)$$

where $f_1 = f_x^u, \dots, f_6 = f_z^w$. With the help of Hooke's law and (8), $\text{div } \boldsymbol{\sigma}$ can be written in terms of the displacement field $\boldsymbol{\gamma}$:

$$\text{div } \boldsymbol{\sigma} = \mathbf{D}(\nabla) \boldsymbol{\gamma}, \quad (\text{div } \boldsymbol{\sigma})_{\alpha} = D_{\alpha\beta}(\nabla) \gamma_{\beta}, \quad (17)$$

$$D_{\alpha\beta}(\nabla) = C_{\alpha i \beta j} \frac{\partial^2}{\partial x_i \partial x_j}. \quad (18)$$

Here, $\gamma_1 = u_x, \dots, \gamma_6 = w_z$. According to (17), the equations of balance (16) result in

$$\mathbf{D}(\nabla) \boldsymbol{\gamma} + \mathbf{f} = \mathbf{0}. \quad (19)$$

Equation (19), $\mathbf{f} = \mathbf{f}^u \oplus \mathbf{f}^w$ and $\boldsymbol{\gamma} = \mathbf{u} \oplus \mathbf{w}$ imply a decomposition of $\mathbf{D}(\nabla)$ into four 3×3 blocks:

$$\mathbf{D}(\nabla) = \begin{bmatrix} \mathbf{D}^{uu}(\nabla) & \mathbf{D}^{uw}(\nabla) \\ \mathbf{D}^{wu}(\nabla) & \mathbf{D}^{ww}(\nabla) \end{bmatrix}. \quad (20)$$

Explicitly, we have¹

$$\begin{aligned} \mathbf{D}^{uu}(\nabla) &= \mu \mathbf{1} \nabla^2 + (\lambda + \mu) \nabla \otimes \nabla, \\ \mathbf{D}^{uw}(\nabla) &= \mathbf{D}^{wu,t}(\nabla) \\ &= \frac{\mu_3}{\sqrt{6}} \begin{bmatrix} F_1(x, y, z) & F_3(x, y) & F_2(x, z) \\ F_2(y, x) & F_1(y, z, x) & F_3(y, z) \\ F_3(z, x) & F_2(z, y) & F_1(z, x, y) \end{bmatrix}, \\ \mathbf{D}^{ww}(\nabla) &= \mu_5 \mathbf{1} \nabla^2 \\ &+ \frac{\mu_4 - \mu_5}{3} \begin{bmatrix} F_4(x, y, z) & F_5(x, y) & F_5(x, z) \\ F_5(y, x) & F_4(y, z, x) & F_5(y, z) \\ F_5(z, x) & F_5(z, y) & F_4(z, x, y) \end{bmatrix}. \end{aligned} \quad (21)$$

¹ Here, some printing errors of reference [6] have been eliminated.

In (21), we have used the abbreviations

$$\begin{aligned}
F_1(a, b, c) &= -\frac{\partial^2}{\partial a^2} - \frac{1}{\tau} \frac{\partial^2}{\partial b^2} + \tau \frac{\partial^2}{\partial c^2}, \\
F_2(a, b) &= -\frac{2}{\tau} \frac{\partial^2}{\partial a \partial b}, \\
F_3(a, b) &= 2\tau \frac{\partial^2}{\partial a \partial b}, \\
F_4(a, b, c) &= \frac{\partial^2}{\partial a^2} + \tau^2 \frac{\partial^2}{\partial b^2} + \frac{1}{\tau^2} \frac{\partial^2}{\partial c^2}, \\
F_5(a, b) &= 2 \frac{\partial^2}{\partial a \partial b}.
\end{aligned} \tag{22}$$

$\tau = \frac{1}{2}(1 + \sqrt{5})$ is the Golden Mean, defined as the positive root of the quadratic equation $x^2 - x - 1 = 0$.

2.2 Green's function of the elastic equations of balance

The solution of (19) for arbitrary body forces \mathbf{f} can be obtained by calculating the integral

$$\gamma(\mathbf{x}) = \int \mathbf{G}(\mathbf{x} - \mathbf{x}') \mathbf{f}(\mathbf{x}') d^3x', \tag{23}$$

where $\mathbf{G}(\mathbf{x} - \mathbf{x}')$ is the elastic Green's function of icosahedral quasicrystals. The constitutive equation for $\mathbf{G}(\mathbf{x})$ is

$$\mathbf{D}(\nabla) \mathbf{G}(\mathbf{x}) + \mathbf{1} \delta(\mathbf{x}) = \mathbf{0}. \tag{24}$$

An approximate solution for $\mathbf{G}(\mathbf{x})$ is given in [6]. Since (21) are the components of $\mathbf{D}(\nabla)$ for linear elasticity, the displacement field provided by (23) is the correct solution only in domains where the linearity conditions are fulfilled.

For the purpose of this work, we only need to know the solution $\mathbf{G}_{00}(\mathbf{x})$ for elastic isotropy in phonon and phason spaces, defined by the conditions $\mu_3 = 0$ and $\mu_4 = \mu_5$. With the well-known elastic Green's function for three-dimensional, isotropic media [2] and the solution of the fundamental Poisson's equation in three dimensions, the exact $\mathbf{G}_{00}(\mathbf{x})$, which reflects decoupled phonon and phason elasticity, is

$$\begin{aligned}
\mathbf{G}_{00}^{uu}(\mathbf{x}) &= \frac{1}{8\pi\mu(\lambda + 2\mu)} \left[(\lambda + 3\mu) \frac{1}{|\mathbf{x}|} \mathbf{1} + (\lambda + \mu) \frac{\mathbf{x} \otimes \mathbf{x}}{|\mathbf{x}|^3} \right], \\
\mathbf{G}_{00}^{ww}(\mathbf{x}) &= \frac{1}{4\pi\mu_5|\mathbf{x}|} \mathbf{1}, \\
\mathbf{G}_{00}^{uw}(\mathbf{x}) &= \mathbf{G}_{00}^{wu}(\mathbf{x}) = \mathbf{0}.
\end{aligned} \tag{25}$$

2.3 Elastic theory of dislocations

A dislocation D is characterized by its non-vanishing line integral

$$\oint_{\partial F_D} d\phi_{\mathbf{k}} = 2\pi m_{\mathbf{k}}, \quad m_{\mathbf{k}} = 0, \pm 1, \pm 2, \dots, \tag{26}$$

along any closed contour ∂F_D surrounding the core of D , which exists in physical space only [16, 17]. Equation (26) guarantees for the continuity of the mass density $\rho(\mathbf{x})$ outside the dislocation core, as can be seen from (1). In case of periodic crystals, the lattice remains unaltered outside the dislocation core. Because of phasons, the same is not true in quasicrystals [18].

From equation (2), condition (26) can be expressed in terms of $\boldsymbol{\kappa}$ and $d\boldsymbol{\gamma}$:

$$\oint_{\partial F_D} \boldsymbol{\kappa} \cdot d\boldsymbol{\gamma} = -2\pi m_{\mathbf{k}}. \tag{27}$$

The six-dimensional Burgers vector is $\mathbf{b} = \mathbf{b}^u \oplus \mathbf{b}^w$, where \mathbf{b}^u , \mathbf{b}^w and \mathbf{b} are defined

$$\mathbf{b}^u = \oint_{\partial F_D} d\mathbf{u}, \quad \mathbf{b}^w = \oint_{\partial F_D} d\mathbf{w}, \quad \mathbf{b} = \oint_{\partial F_D} d\boldsymbol{\gamma}. \tag{28}$$

This allows us to rewrite (27) in the form

$$\boldsymbol{\kappa} \cdot \mathbf{b} = \mathbf{k}^{\parallel} \cdot \mathbf{b}^u + \mathbf{k}^{\perp} \cdot \mathbf{b}^w = -2\pi m_{\mathbf{k}}. \tag{29}$$

As a conclusion from (3) and (29), \mathbf{b} must be a vector of the direct hyperlattice. The irrational orientations of E^{\parallel} and E^{\perp} in hyperspace provide non-vanishing components \mathbf{b}^u and \mathbf{b}^w for every dislocation.

Because of equations (28), the displacement fields of dislocations are multiple-valued, and therefore not integrable. According to potential theory, the non-integrability of equations (5) corresponds to $\text{curl } \boldsymbol{\beta}^{u,w} \neq \mathbf{0}$. From Stokes' theorem,

$$\begin{aligned}
\mathbf{b}^{u,w} &= \oint_{\partial F_D} d(\mathbf{u}, \mathbf{w}) = \oint_{\partial F_D} \boldsymbol{\beta}^{u,w} d\mathbf{x} \\
&= \int_{F_D} \text{curl } \boldsymbol{\beta}^{u,w} d\mathbf{f} = \int_{F_D} \boldsymbol{\alpha}^{u,w} d\mathbf{f},
\end{aligned} \tag{30}$$

where the surface integrals extend over the surface F_D , bounded by ∂F_D and pierced by the dislocation D . Because of equation (30), the tensors $\boldsymbol{\alpha}^{u,w}$ are dislocation densities in phonon and phason spaces per area of physical space. It is

$$\boldsymbol{\alpha}^{u,w} = \text{curl } \boldsymbol{\beta}^{u,w}, \quad \alpha_{ij}^{u,w} = \epsilon_{jkl} \frac{\partial \beta_{il}^{u,w}}{\partial x_k}. \tag{31}$$

Equations (31), in connection with boundary conditions to be fulfilled, are the defining equations for $\boldsymbol{\beta}^{u,w}$.

By means of equations (6), the elastic distortion fields $\boldsymbol{\beta}^{u,w}$ lead to the strain fields $\boldsymbol{\varepsilon}^{u,w}$. Connected with the elastic strain fields of dislocations are stress fields (10). In the absence of body forces \mathbf{f} , they must fulfill equation (16) in the form

$$\text{div } \boldsymbol{\sigma} = \mathbf{0}. \tag{32}$$

3 Solving the problem of a single dislocation

Elastic fields fulfilling equations (10, 28) and (32) simultaneously constitute the solution of the dislocation problem.

Note that equations (28) for a single dislocation are a special case of the general situation, which is characterized by an incompatibility field [19]. The projection method [20] is a possibility to solve the dislocation problem. A summary, containing the description of several other methods, is given in [21].

3.1 The projection method

The idea of the projection method is the following. In a first step, an arbitrary, multiple-valued displacement field $\hat{\gamma} = \hat{\mathbf{u}} \oplus \hat{\mathbf{w}}$ fulfilling (28),

$$\mathbf{b}^u = \oint_{\partial F_D} d\hat{\mathbf{u}}, \quad \mathbf{b}^w = \oint_{\partial F_D} d\hat{\mathbf{w}}, \quad \mathbf{b} = \oint_{\partial F_D} d\hat{\gamma}, \quad (33)$$

has to be found. According to equation (5), this displacement field leads to distortions, and from (6) the corresponding eigenstrains $\hat{\varepsilon}^{u,w}$ can be calculated. But the eigenstress field $\hat{\sigma} = \mathbf{C} \hat{\varepsilon}$ will not be compatible with the equations of balance (32) in general. There may exist a divergence $\text{div } \hat{\sigma} \neq \mathbf{0}$.

In the second step, a single-valued displacement field $\tilde{\gamma} = \tilde{\mathbf{u}} \oplus \tilde{\mathbf{w}}$, leading to strain fields $\tilde{\varepsilon}^{u,w}$ and stresses $\tilde{\sigma} = \mathbf{C} \tilde{\varepsilon}$, due to equations (8) and (10), respectively, has to be found. $\tilde{\gamma}$ has to be determined in such a way, that the divergence of the total stress field $\sigma = \hat{\sigma} + \tilde{\sigma}$ vanishes:

$$\text{div } \sigma = \text{div } (\hat{\sigma} + \tilde{\sigma}) = \mathbf{0}. \quad (34)$$

In this step, the stress field $\hat{\sigma}$ is *projected* from the space of stress fields with arbitrary divergence onto the space of stresses with vanishing divergence. The result of this projection is the true stress field σ . Since the displacement field $\tilde{\gamma}$ is single-valued, we have

$$\oint_{\partial F_D} d\tilde{\mathbf{u}} = \mathbf{0}, \quad \oint_{\partial F_D} d\tilde{\mathbf{w}} = \mathbf{0}, \quad \oint_{\partial F_D} d\tilde{\gamma} = \mathbf{0}. \quad (35)$$

Finally, the elastic fields of the dislocation are

$$\gamma = \hat{\gamma} + \tilde{\gamma}, \quad \varepsilon = \hat{\varepsilon} + \tilde{\varepsilon}, \quad \sigma = \hat{\sigma} + \tilde{\sigma}. \quad (36)$$

Equation (10) is satisfied because we have used $(\hat{\sigma}, \tilde{\sigma}) = \mathbf{C}(\hat{\varepsilon}, \tilde{\varepsilon})$. (28) is fulfilled because of equations (33) and (35). (32) is true due to equation (34). γ is multiple-valued because $\hat{\gamma}$ is, whereas ε and σ are single-valued.

The problem of finding the right $\tilde{\gamma}$ can be solved as described below. The equations of balance (19) read for the case of the displacement field $\tilde{\gamma}$

$$\mathbf{D}(\nabla) \tilde{\gamma} + \check{\mathbf{f}} = \mathbf{0}, \quad (37)$$

where $\mathbf{D}(\nabla) \tilde{\gamma} = \text{div } \tilde{\sigma}$. Comparing (37) with equation (34) leads to the identification

$$\check{\mathbf{f}} = \text{div } \hat{\sigma} \quad (38)$$

for the right $\check{\mathbf{f}}$ to be used as fictitious body force in (37) in order to calculate $\tilde{\gamma}$. Therefore, in the second step of the projection method, the equations of balance

$$\mathbf{D}(\nabla) \tilde{\gamma} + \text{div } \hat{\sigma} = \mathbf{0} \quad (39)$$

have to be solved. We want to stress that the body force $\check{\mathbf{f}} = \text{div } \hat{\sigma}$ is not a real force.

The projection method amounts to adding a singular displacement field and a non-singular one in order to satisfy equation (32), which is not yet fulfilled after the first step. The splitting up into a singular and a non-singular part and the introduction of local axes, as done below, has already been discussed in [16].

3.2 Symmetry-adapted coordinate systems

In this paper, we consider straight dislocations D having two-, three- and fivefold line directions. For simplicity, a coordinate system K_D^u with its z^u -axis parallel to the respective dislocation line of D should be used in physical space. There arise certain symmetries from phasonic Burgers vectors, which can be seen clearly when additionally choosing the z^w -axis of the new coordinate system K_D^w in phason space parallel to that symmetry axis, which corresponds to the line direction in physical space.

The difference between the two-, three- and fivefold dislocation lines lies in different components of the elastic tensor \mathbf{C} . The components $C_{\alpha i \beta j}$ resulting from (9, 14) belong to the coordinate systems of Figures 1, 2, which are appropriate coordinate systems for twofold dislocations. The components $C_{D, \alpha i \beta j}$ of the elastic tensors in symmetry-adapted coordinate systems for the three- and fivefold dislocations are obtained by coordinate transformations.

Consider orthogonal transformations in phonon and phason spaces,

$$v_{D,i}^u = \Gamma_{D,ij}^u v_j^u, \quad v_{D,i}^w = \Gamma_{D,ij}^w v_j^w, \quad (40)$$

connecting the components of the vector \mathbf{v} in the symmetry-adapted coordinate systems with its components belonging to the coordinate systems of Figures 1, 2. The transformations of the strain components are then

$$\varepsilon_{D,ij}^u = \Gamma_{D,ik}^u \Gamma_{D,jl}^u \varepsilon_{kl}^u, \quad \varepsilon_{D,ij}^w = \Gamma_{D,ik}^w \Gamma_{D,jl}^w \varepsilon_{kl}^w. \quad (41)$$

Explicitly, we have taken

$$\begin{aligned} \mathbf{\Gamma}_3^u &= c_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & \tau^2 & -1 \\ 0 & 1 & \tau^2 \end{bmatrix}, & \mathbf{\Gamma}_3^w &= c_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\tau^2 \\ 0 & \tau^2 & 1 \end{bmatrix}, \\ \mathbf{\Gamma}_5^u &= c_2 \begin{bmatrix} \tau & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & \tau \end{bmatrix}, & \mathbf{\Gamma}_5^w &= c_2 \begin{bmatrix} 1 & 0 & \tau \\ 0 & 1 & 0 \\ -\tau & 0 & 1 \end{bmatrix}, \end{aligned} \quad (42)$$

as orthogonal transformation matrices in (40). They result from choosing the directions $\mathbf{P}^{\parallel}(\mathbf{e}_3 + \mathbf{e}_4 - \mathbf{e}_6)$ and $\mathbf{P}^{\parallel} \mathbf{e}_3$, respectively, as dislocation lines in Figure 1. The coefficients c_1, c_2 are

$$c_1 = \frac{1}{\sqrt{1 + \tau^4}}, \quad c_2 = \frac{1}{\sqrt{1 + \tau^2}}. \quad (43)$$

When substituting the components $\varepsilon_{ij}^{u,w}$ of equation (9) by components $\varepsilon_{D,ij}^{u,w}$, due to the inversion of equations (40), the components $C_{D,\alpha i \beta j}$ are obtained.

The positions in phonon space are best described by cylindrical coordinates r and ϕ , beside the Cartesian coordinates x, y in the symmetry-adapted coordinate systems. From now on, we use the notation $\mathbf{x} = [x, y]^t$ for the position perpendicular to the dislocation lines.

3.3 Generalized differentiation and its application to the projection method

The best $\hat{\gamma}$ to start with in the first step of the projection method is

$$\hat{\gamma} = \frac{\mathbf{b}}{2\pi} \phi. \quad (44)$$

The resulting distortion and strain fields are

$$\hat{\varepsilon}^w = \hat{\beta}^{u,w} = \frac{1}{2\pi(x^2 + y^2)} \begin{bmatrix} -b_1^{u,w} y & b_1^{u,w} x & 0 \\ -b_2^{u,w} y & b_2^{u,w} x & 0 \\ -b_3^{u,w} y & b_3^{u,w} x & 0 \end{bmatrix}, \quad (45)$$

$$\hat{\varepsilon}^u = \frac{1}{4\pi(x^2 + y^2)} \begin{bmatrix} -2b_1^u y & b_1^u x - b_2^u y & -b_3^u y \\ b_1^u x - b_2^u y & 2b_2^u x & b_3^u x \\ -b_3^u y & b_3^u x & 0 \end{bmatrix}.$$

The corresponding dislocation densities $\hat{\alpha}^{u,w}$ (31) are $\mathbf{0}$ for $\mathbf{x} \neq \mathbf{0}$. To consider the behaviour at $\mathbf{x} = \mathbf{0}$, where no partial derivatives in classical sense are defined, one has to assume all functions to be generalized functions and calculate the generalized partial derivatives [22]. Note that, because of (44) and (45), the linear elasticity breaks down below a finite cut-off distance from the dislocation line.

In case of homogeneous functions f of degree -1 in two variables x, y , the generalized partial derivatives are

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial x} \Big|_G + \delta(\mathbf{x}) \oint_{\partial G} f \, dy, \quad (46)$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial y} \Big|_G - \delta(\mathbf{x}) \oint_{\partial G} f \, dx,$$

where the respective first expressions represent certain generalized functions connected with the classical partial derivatives. G is any bounded region containing the origin $\mathbf{x} = \mathbf{0}$. Equations (46) indicate that there may be δ -functions on the dislocation lines. Their respective weight may depend on the choice of G , but becomes independent of G when considering any combination of generalized partial derivatives with the total classical derivative vanishing.

Calculating the dislocation densities (31) results in

$$\begin{aligned} \hat{\alpha}_{ij}^{u,w} &= \delta_{j3} \delta(\mathbf{x}) \oint_{\partial G} [\hat{\beta}_{i1}^{u,w} dx + \hat{\beta}_{i2}^{u,w} dy] \\ &= \delta_{j3} \frac{b_i^{u,w}}{2\pi} \delta(\mathbf{x}) \oint_{\partial G} \left[\frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy \right] \\ &= \delta_{j3} \frac{b_i^{u,w}}{2\pi} \delta(\mathbf{x}) \oint_{\partial G} d\phi = \delta_{j3} b_i^{u,w} \delta(\mathbf{x}). \end{aligned} \quad (47)$$

Therefore, the dislocation densities are point-like,

$$\hat{\alpha}^{u,w} = \delta(\mathbf{x}) \left[\mathbf{0}, \mathbf{0}, \mathbf{b}^{u,w} \right]. \quad (48)$$

According to (35), $\check{\alpha}^{u,w} \equiv \mathbf{0}$.

From equations (10) and (45), the stress field $\hat{\sigma}$ entering the projection method in the second step is homogeneous of degree -1 . Therefore, equations (46) apply when calculating $\text{div } \hat{\sigma}$.

In the second step of the projection method, the solution of (39) is split into further two steps. In a first step, (39) is solved for $\mathbf{x} \neq \mathbf{0}$. This means that only the classical derivatives $(\text{div } \hat{\sigma})|_{\mathbf{x} \neq \mathbf{0}}$ enter (39). Denoting the solution γ' , equation (39) becomes for $\mathbf{x} \neq \mathbf{0}$

$$\mathbf{D}(\nabla) \gamma' + \text{div } \hat{\sigma} = \mathbf{0}. \quad (49)$$

The displacement field γ' leads to the strain field ε' and the stress field σ' , due to (8) and (10). The divergence of the stress field $\hat{\sigma} + \sigma'$ will vanish when considering classical derivatives only, but may still have components proportional to $\delta(\mathbf{x})$. In a second step, these point-like stress sources have to be compensated. With $\text{div}(\hat{\sigma} + \sigma') = \delta(\mathbf{x}) \mathbf{f}_L''$, equation (39) becomes

$$\mathbf{D}(\nabla) \gamma'' + \delta(\mathbf{x}) \mathbf{f}_L'' = \mathbf{0}. \quad (50)$$

Here, \mathbf{f}_L'' is a constant vector having the unit of a force per length. The solution γ'' leads to the strain field ε'' and the stress field σ'' . The final results entering equations (36) are

$$\check{\gamma} = \gamma' + \gamma'', \quad \check{\varepsilon} = \varepsilon' + \varepsilon'', \quad \check{\sigma} = \sigma' + \sigma''. \quad (51)$$

In a short excursion, we want to discuss the meaning of the divergence $\delta(\mathbf{x}) \mathbf{f}_L''$ of the stress tensor on the dislocation lines. According to (46),

$$f_{L,\alpha}'' = \oint_{\partial G} [(\hat{\sigma} + \sigma')_{\alpha 1} dy - (\hat{\sigma} + \sigma')_{\alpha 2} dx]. \quad (52)$$

(52) is the α -component of

$$\mathbf{t}_L'' = \oint_{\partial G} \mathbf{t}'' \, ds = \oint_{\partial G} (\hat{\sigma} + \sigma') \mathbf{n} \, ds, \quad (53)$$

where \mathbf{t}'' is the six-dimensional surface force remaining after the divergence of the stress tensor in terms of classical derivatives has been brought to zero. \mathbf{t}_L'' represents the net force per length of the z^u -axis acting on the interior of G , which must vanish [23].

3.4 Recursion formulae

Unfortunately, there is no possibility to calculate $\tilde{\gamma}$ in the second step of the projection method exactly. We have expanded the elastic fields into perturbation series providing an approximate solution of the dislocation problem, the zeroth order being the solution for the case of elastic isotropy and the higher orders the perturbation arising from the deviation from isotropy. Closely following the projection method, the solution of the recursion formulae is the summation of the singular displacement field of zeroth order and non-singular displacement fields of higher order. This kind of dealing with anisotropy has already been used in connection with Green's functions of crystals [24] and quasicrystals [6] and to calculate the fields of dislocations [24] and cracks [25]. [23] comprises a more enclosing approach to the handling with elastic anisotropy.

The zeroth order is the solution for elastic isotropy ($\mu_3 = 0$ and $\mu_4 = \mu_5$), which is known (see Appendix B). The elastic fields can be expanded with respect to the variables μ_3 and $\mu_4 - \mu_5$. We shall mark any physical quantity f being proportional to $\mu_3^m (\mu_4 - \mu_5)^n$ by lower indices mn : $f_{mn} \sim \mu_3^m (\mu_4 - \mu_5)^n$.

From (21), it is obvious that

$$\mathbf{D}(\nabla) = \mathbf{D}_{00}(\nabla) + \mathbf{D}_{10}(\nabla) + \mathbf{D}_{01}(\nabla), \quad (54)$$

where according to equations (21)

$$\mathbf{D}_{00}(\nabla) = \begin{bmatrix} \mu \mathbf{1} \nabla^2 + (\lambda + \mu) \nabla \otimes \nabla & \mathbf{0} \\ \mathbf{0} & \mu_5 \mathbf{1} \nabla^2 \end{bmatrix}. \quad (55)$$

Because of (18), the decomposition (54) corresponds to the following decomposition of the elastic tensor \mathbf{C} :

$$\mathbf{C} = \mathbf{C}_{00} + \mathbf{C}_{10} + \mathbf{C}_{01}. \quad (56)$$

For the elastic fields, the perturbation series read

$$\gamma = \sum \gamma_{mn}, \quad \varepsilon = \sum \varepsilon_{mn}, \quad \sigma = \sum \sigma_{mn}. \quad (57)$$

The conditions, which the different orders must fulfill, are the following. First, all displacement fields except for zeroth order must be single-valued:

$$\mathbf{b} = \oint_{\partial F_D} d\gamma_{00}, \quad \mathbf{0} = \oint_{\partial F_D} d\gamma_{mn} \quad (mn \neq 00). \quad (58)$$

This is because \mathbf{b} belongs to zeroth order. Second, Hooke's law (10) must connect strains and stresses in all orders:

$$\begin{aligned} \sigma_{00} &= \mathbf{C}_{00} \varepsilon_{00}, \\ \sigma_{m0} &= \mathbf{C}_{00} \varepsilon_{m0} + \mathbf{C}_{10} \varepsilon_{m-1,0}, \\ \sigma_{0n} &= \mathbf{C}_{00} \varepsilon_{0n} + \mathbf{C}_{01} \varepsilon_{0,n-1}, \\ \sigma_{mn} &= \mathbf{C}_{00} \varepsilon_{mn} + \mathbf{C}_{10} \varepsilon_{m-1,n} + \mathbf{C}_{01} \varepsilon_{m,n-1}. \end{aligned} \quad (59)$$

Here, the last three equations are valid for $m > 0$, $n > 0$ and both $m, n > 0$, respectively. Third, the divergence of the stress field of each order must vanish:

$$\operatorname{div} \sigma_{mn} = \mathbf{0}. \quad (60)$$

The constitutive equations (58, 59) and (60) can be solved recursively using the projection method. At this, the zeroth order must be treated somewhat different than higher orders.

Note that $\hat{\gamma}$ and $\hat{\varepsilon}$ given by equations (44) and (45) belong to zeroth order, as the stress field $\hat{\sigma}_{00} = \mathbf{C}_{00} \hat{\varepsilon}$. $\operatorname{div} \sigma_{00} = \mathbf{0}$ must be valid, and therefore the projection method requires the solution of the equations of balance

$$\mathbf{D}_{00}(\nabla) \tilde{\gamma}_{00} + \underbrace{\operatorname{div}(\mathbf{C}_{00} \hat{\varepsilon})}_{=\hat{\mathbf{f}}_{00}} = \mathbf{0}. \quad (61)$$

When omitting the lower indices, this is exactly the procedure of Section 3.1. The solution of (61) leads to the strain field $\check{\varepsilon}_{00}$ according to equations (8). Finally, we have

$$\gamma_{00} = \check{\gamma}_{00} + \hat{\gamma}, \quad \varepsilon_{00} = \check{\varepsilon}_{00} + \hat{\varepsilon}, \quad \sigma_{00} = \mathbf{C}_{00}(\check{\varepsilon}_{00} + \hat{\varepsilon}). \quad (62)$$

The full γ_{00} is given in Appendix B.

We demonstrate the procedure in case of higher orders for $m0 \neq 00$ only. The approach in the other cases is completely analogous. When calculating the elastic fields of order $m0$, the solutions of all orders $\tilde{m}0$ with $\tilde{m} < m$ have already been determined. The condition for the stress field σ_{m0} to be fulfilled is $\operatorname{div} \sigma_{m0} = \mathbf{0}$, where σ_{m0} is determined by the second equation (59). Obviously, the solution of the equations of balance

$$\mathbf{D}_{00}(\nabla) \gamma_{m0} + \underbrace{\operatorname{div}(\mathbf{C}_{10} \varepsilon_{m-1,0})}_{=\mathbf{f}_{m0}} = \mathbf{0} \quad (63)$$

provides the displacement field γ_{m0} of order $m0$. Equation (63) is obtained immediately by the action of the differential operator div on both sides of the second equation (59) and the fact that $\mathbf{D}_{00}(\nabla) \gamma_{m0} = \operatorname{div}(\mathbf{C}_{00} \varepsilon_{m0})$, with γ_{m0} and ε_{m0} connected by equations (8).

Concerning the perturbation expansions of the fields $\check{\gamma}$, $\check{\varepsilon}$, $\check{\sigma}$ and $\check{\mathbf{f}}$ introduced in Section 3.1, we have $\gamma_{mn} = \check{\gamma}_{mn}$ and $\varepsilon_{mn} = \check{\varepsilon}_{mn}$ except for zeroth order, where (62) must be applied. The relation $\sigma_{mn} = \check{\sigma}_{mn}$ is true for orders $m+n > 1$, whereas σ_{00} , σ_{10} and σ_{01} consist of parts belonging to $\hat{\sigma}$ and $\check{\sigma}$. The expansion of $\check{\mathbf{f}}$ comprises the three terms $\check{\mathbf{f}}_{00}$, $\check{\mathbf{f}}_{10}$ and $\check{\mathbf{f}}_{01}$ according to (38) and (56), and therefore \mathbf{f}_{m0} in (63) is a completely different fictitious body force. For these reasons, the $\check{\cdot}$ -notation of the projection method is not appropriate in case of equation (63).

As an important result of the above considerations, the perturbation expansions of the elastic fields can be calculated by solving the equations of balance with the differential operator $\mathbf{D}_{00}(\nabla)$ instead of the full $\mathbf{D}(\nabla)$, a task which proves to be relatively easy. We have performed our calculations with the help of MapleV², and made use of the method described in Section 3.3. Therefore, all displacement fields are compounded by two parts: $\tilde{\gamma}_{mn} = \gamma'_{mn} + \gamma''_{mn}$ for all mn .

² MapleV Release 4 ©1981-1996 by Waterloo Maple Inc. and MapleV Release 5.1 ©1981-1998 by Waterloo Maple Inc.

3.5 Solving the recursion formulae

The calculation of the displacement fields γ'_{mn} can make use of the fact that they depend on ϕ only:

$$\gamma'_{mn}(\mathbf{x}) \equiv \gamma'_{mn}(\phi), \quad (64)$$

with each component $\gamma'_{mn,\alpha} = c_{mn,\alpha p} e^{ip\phi}$ being a real combination of complex harmonics. Therefore, things are much easier when expressing all derivatives (55) in terms of $\partial/\partial r$, $\partial/\partial\phi$ and $\partial/\partial z$, with $\partial/\partial r$ and $\partial/\partial z$ vanishing when applied to the displacement fields (64).

Transforming $\mathbf{D}_{00}(\nabla)$ yields the equations of balance of zeroth order in the form

$$\begin{aligned} \begin{bmatrix} -(\lambda + 2\mu) + \mu \frac{\partial^2}{\partial\phi^2} & -(\lambda + 3\mu) \frac{\partial}{\partial\phi} \\ (\lambda + 3\mu) \frac{\partial}{\partial\phi} & -\mu + (\lambda + 2\mu) \frac{\partial^2}{\partial\phi^2} \end{bmatrix} \begin{bmatrix} u'_r \\ u'_\phi \end{bmatrix} + \begin{bmatrix} \bar{f}_r^u \\ \bar{f}_\phi^u \end{bmatrix} = \mathbf{0}, \\ \mu \frac{\partial^2}{\partial\phi^2} u'_z + \bar{f}_z^u = 0, \\ \mu_5 \frac{\partial^2}{\partial\phi^2} u'_k + \bar{f}_k^w = 0, \end{aligned} \quad (65)$$

where $k \in \{x, y, z\}$. From (45), all possible $(\text{div} \dots)|_{\mathbf{x} \neq \mathbf{0}}$ in equations (61, 63) and in the analogous equations for other orders depend on r like r^{-2} , and in (65) we use the notation $(\text{div} \dots)|_{\mathbf{x} \neq \mathbf{0}} = \frac{1}{r^2} \bar{\mathbf{f}}$, where the length force $\bar{\mathbf{f}}$ depends on ϕ only. Equations (65) justify the ansatz (64). The order indices are omitted here.

In the second step of the calculation of $\tilde{\gamma}_{mn}$, the divergence of the stress tensor on the dislocation line must be brought to zero. This leads to the additional displacement field γ''_{mn} entering $\tilde{\gamma}_{mn}$. To perform this second step, the fields γ''_α resulting from (50) with the prototypical forces $\mathbf{f}''_{L\alpha}$ defined by $f''_{L\alpha,\beta} = \delta_{\alpha\beta}$ must be available. We have calculated these γ''_α with the help of (23) for zeroth order. They are given in Appendix B. From there it is obvious that $\ln r$ -terms and hereby dependencies on r join the displacement fields.

For the purpose of this paper, we have calculated the elastic displacement, strain and stress fields of two- and threefold dislocations up to orders mn where $m + n \leq 5$, and for fivefold dislocations up to $m + n \leq 15$.

For fivefold dislocations and vanishing phonon-phason-coupling, the elastic fields are known in closed form [26]. When we neglect the phonon-phason-coupling in our algorithm, then our analytical expressions agree with an expansion of this closed solution into a perturbation series in $\mu_4 - \mu_5$ up to all calculated orders. But also our algorithm clearly shows, that neither a closed solution is possible for finite phonon-phason-coupling nor for other directions of the dislocation line.

The solution of [26] has been obtained by the more frequently used generalized Green's method. The calculated displacements are applied to atomic models of dislocations along a fivefold direction of i-AIPdMn to obtain dislocation-induced atomic positions. As we shall prove in

Section 4.2, the true fivefold symmetry of the displacement fields is exclusively induced by the phonon-phason-coupling, but investigating the effect of the phonon-phason-coupling on the atomic positions is beyond the scope of this paper.

4 Results and discussion

4.1 General results

The strain and stress fields of all orders behave like $\frac{1}{r}$, with r being the distance from the dislocation line. This is exactly compatible with what one would expect from the exact solution, provided *e.g.* by the projection method, and is also compatible with results from numerical methods.

Apart from zeroth order, the displacement fields show positive parity perpendicular to the dislocation line:

$$\gamma_{mn}(-\mathbf{x}) = \gamma_{mn}(\mathbf{x}). \quad (66)$$

In contrast to this, the strain and stress fields of all orders exhibit negative parity:

$$\varepsilon_{mn}(-\mathbf{x}) = -\varepsilon_{mn}(\mathbf{x}), \quad \sigma_{mn}(-\mathbf{x}) = -\sigma_{mn}(\mathbf{x}). \quad (67)$$

These properties follow from the equations of balance (16) and (19), respectively, when using the fact that all fictitious forces occurring in the projection method have positive parity. Note that (67) guarantees for the total torque acting on the dislocation core to vanish.

The components $\varepsilon_{mn,33}^u$ and $\varepsilon_{mn,33}^w$ of the strain tensors vanish. This is a consequence of the infinite geometry. Except for the case of twofold screw dislocations, $\varepsilon_{mn,33}^u = \varepsilon_{mn,33}^w \equiv 0$ is not compatible with $\sigma_{mn,33}^u \equiv 0$ and $\sigma_{mn,33}^w \equiv 0$. Therefore, stresses are present parallel to the dislocation lines. It is not quite clear how to interpret these statements in phason space.

The simplest dislocations are the twofold ones. Twofold edge dislocations induce only displacements perpendicular to the dislocation line, and screw dislocations only parallel to the dislocation line. In case of the other line directions, Burgers vectors and displacements perpendicular and parallel to the dislocation lines are no longer decoupled.

For every order mn where m is even, the phononic displacement, strain and stress fields depend linearly on \mathbf{b}^u only, whereas the phasonic fields depend on \mathbf{b}^w only. The contrary is true for any order mn , where m is odd. Additionally, we have $\mathbf{u}_{0n} \equiv \mathbf{0}$, $\varepsilon_{0n}^u \equiv \mathbf{0}$ and $\sigma_{0n}^u \equiv \mathbf{0}$ for all $n > 0$.

In icosahedral quasicrystals, it is, in general, not possible to compute the elastic fields belonging to a Burgers vector arising from \mathbf{b} by rotation about the dislocation line from the fields belonging to \mathbf{b} by the same rotation. This method can, for example, be applied to pentagonal quasicrystals [4].

4.2 Displacement fields of fivefold dislocations

The following performances refer to the fivefold coordinate systems introduced in Section 3.2. The classification into phasonic edge and screw dislocations is problematic in some respects [16]. To our opinion, this discrimination makes sense, because only phasonic Burgers vectors which are parallel to the z -axes of the coordinate systems of Section 3.2 do not break the n -fold symmetries induced by phasonic n -fold screw dislocations.

The higher displacement corrections shown in the next two subsections are computed on the circle $\sqrt{x^2 + y^2} = 10b$ in the xy -plane. Here, b is the length of the different Burgers vectors we have assumed (see Eqs. (68, 69)). We have chosen this circle, because for our choice of elastic constants, this is the lower limit for no strain tensor component to exceed an absolute value of 0.1, which we regard as limit for the validity of linear elasticity. In the diagrams with displacement components u_z parallel to the dislocation line, the label L stands for the arc length of this circle. All displacement fields are standardized to have a vanishing net displacement on the circle, which has been achieved by adding suitable constant displacement fields.

For the calculation of the elastic fields, the elastic constants of i-AlPdMn have been used. The phasonic elastic constants are $\lambda = 85$ GPa and $\mu = 65$ GPa [13]. For the phasonic elastic constants, we have taken the values $K_1/kT = 0.1/\text{atom}$ and $K_2/kT = -0.05/\text{atom}$ and supposed a quenching temperature of 500°C [14]. This leads to our elastic constants $\mu_4 = 0.012$ GPa and $\mu_5 = 0.12$ GPa. The phonon-phason-coupling has been supposed to be $\mu_3 = 1$ GPa.

Note that the displacements alone are no good quantities to measure the elastic deformation qualitatively, but the strains are. Note also, that the phasonic displacement corrections are very small compared to the phasonic Burgers vectors, and that all the corrections shown here vanish with the phonon-phason-coupling μ_3 .

4.2.1 Fivefold edge dislocation

We have chosen a six-dimensional, prototypical Burgers vector

$$\mathbf{b}^{u,w} = [0, b, 0]^t. \quad (68)$$

For the length of the phasonic part \mathbf{b}^u , 1 \AA is the right order of magnitude, whereas under plastic deformation the phasonic part \mathbf{b}^w increases and becomes up to 100 times larger than \mathbf{b}^u [1]. Pure edge or screw dislocations appear very rarely in reality. Due to the edge type of the dislocation defined by (68), the fivefold symmetry of the dislocation line is broken, as can be seen from the displacement, strain and stress fields.

Figures 3 and 4 show the xy -components of the phasonic displacements of order $mn = 10$ and $mn = 20$. They contribute most to the total correction of the phasonic xy -displacement field, which is shown in Figure 5. Obviously, the superposition of these two low

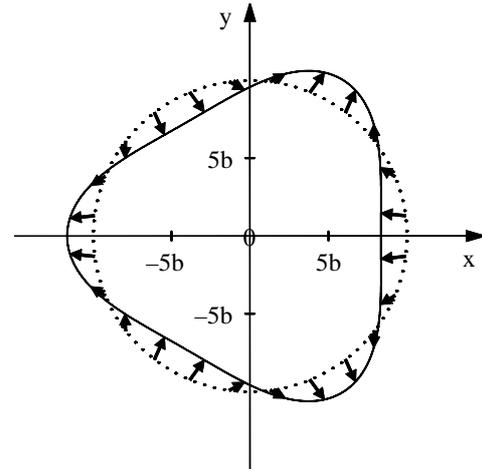


Fig. 3. Phasonic xy -displacement field of the edge dislocation (68), order $mn = 10$. Magnification of the displacement vectors: 4000.

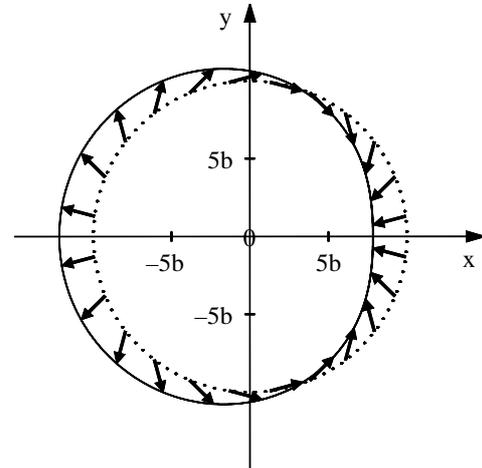


Fig. 4. Phasonic xy -displacement field of the edge dislocation (68), order $mn = 20$. Magnification of the displacement vectors: 6000.

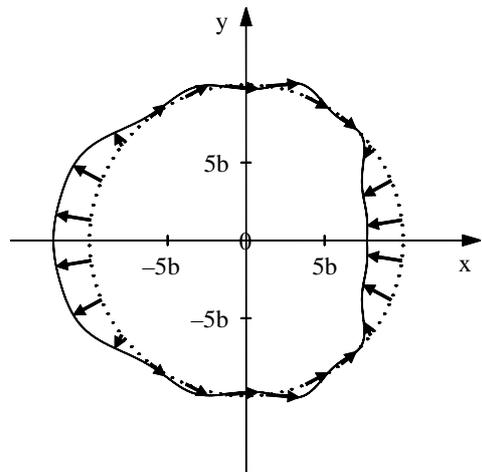


Fig. 5. Phasonic xy -displacement field of the edge dislocation (68), all orders mn with $m + n \leq 15$ except zeroth order. Magnification of the displacement vectors: 2500.

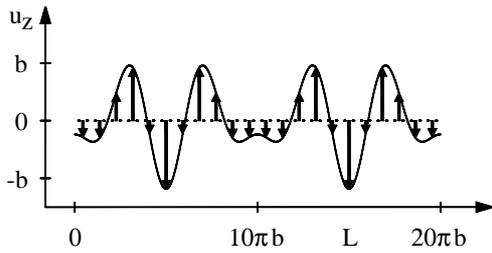


Fig. 6. Phononic z -displacement field of the edge dislocation (68), order $mn = 20$. Magnification of the arrows: 1200.

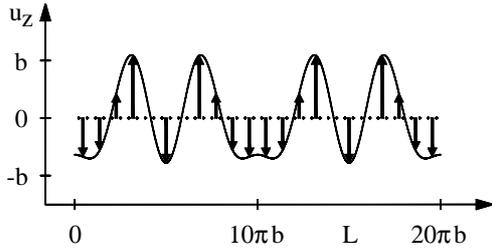


Fig. 7. Phononic z -displacement field of the edge dislocation (68), all orders mn with $m + n \leq 15$. Magnification of the arrows: 2000.

orders already provides a good approximation for the full correction.

In Figures 6 and 7, the z -components of order $mn = 20$ and of all orders mn with $m + n \leq 15$ are shown. Again, the orders $mn = 10$ and $mn = 20$ give the essential contribution to the full displacement field. In zeroth order, no z -component is present. The z -component of order $mn = 10$ is not shown here. It proves to have a negative $\cos 2\phi$ -dependence, which in 2000-fold magnification has a similar absolute amplitude as the components of Figure 6.

The perfect twofold symmetry of the z -components is remarkable. This is due to the condition (66), which the displacement fields have to fulfill. Note that the components of Figures 3–5 fulfill (66) also. In addition to this symmetry, the displacement fields show mirror symmetry with respect to the xz -plane. As an evident explanation, the Volterra cut procedure [17,26] should be performed symmetrically with respect to a cut in the physical xz -plane, so that this plane remains a mirror plane even after the introduction of the dislocation (see Figs. 1, 2). Our results show that the phasonic fields, which have to be subjected to the associated orthogonal space symmetry operation, also have this symmetry, as it must be.

The volume contraction $\frac{\Delta V}{V} = \text{tr}(\epsilon^u)$ and the eigenvalues of the phasonic stress tensor σ^u of zeroth order do not change substantially from the contribution of higher orders.

When considering phasonic components, the typical displacements are more than a hundred times larger than their phononic counterparts. The typical phasonic strains result to be ten times larger than the phononic strains.

We have investigated the convergence behaviour of our perturbation expansion and also calculated the exact displacement fields by the numerical Eshelby's method [20,21]. From there, the correction displacement

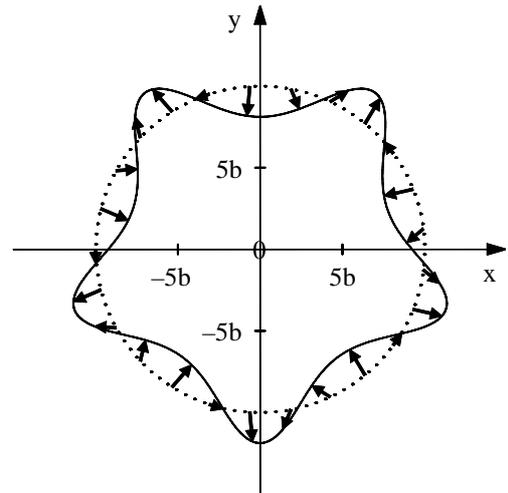


Fig. 8. Phononic xy -displacement field of the screw dislocation (69), order $mn = 20$. Magnification of displacement vectors: 2500.

fields of Figures 5 and 7 are very close to the exact ones. The same is true for the correction displacement field for the fivefold screw dislocation, which is discussed below.

4.2.2 Fivefold screw dislocation

The Burgers vector of a screw dislocation has been chosen to be

$$\mathbf{b}^{u,w} = [0, 0, b]^t. \quad (69)$$

A screw dislocation induces no symmetry breaking parallel to the dislocation line. Therefore, the fivefold symmetry should be recognizable from the phasonic as from the phasonic displacement fields.

From Figure 8, the fivefold symmetry of the phonon displacement field is obvious. Again, $mn = 20$ is the order which provides the largest contribution to the complete xy -displacement field, which is shown in Figure 9. Although the displacement fields look qualitatively very similar, slight differences are present in their functional dependence on \mathbf{x} . No z -component is present in order $mn = 20$.

In case of phason displacements, the fivefold symmetry is not easy to recognize. Figure 10 shows the phasonic displacement field of order $mn = 10$, which provides the largest phasonic xy -displacements occurring in any order. Again, no z -component is present. Note the small magnification, indicating the magnitude of the phason displacements, which are appreciable compared with the length of the phasonic Burgers vector. The position vectors used in Figure 10 refer to the physical coordinate system of Figure 1, but the components of the displacement vectors belong to the phason coordinate system of Figure 2. Looking at the indices of the projected hyperspace basis vectors \mathbf{e}_α in Figures 1 and 2, it is clear, that a rotation about angle $\frac{2\pi}{5}$ in physical space corresponds to a $-\frac{4\pi}{5}$ -rotation in phason space. Therefore, fivefold invariance of

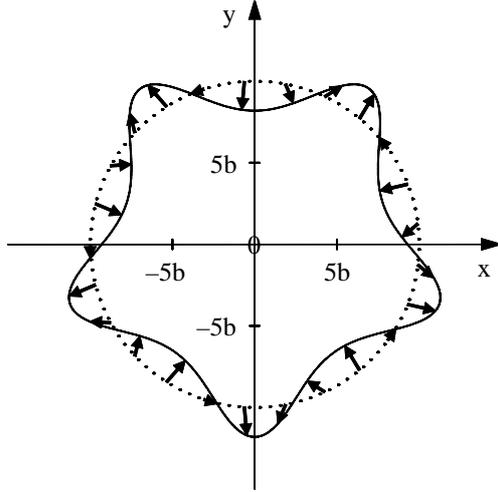


Fig. 9. Phononic xy -displacement field of the screw dislocation (69), all orders mn with $m + n \leq 15$. Magnification of displacement vectors: 1500.

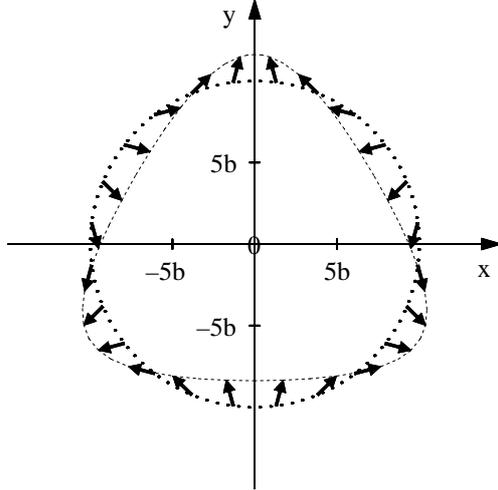


Fig. 10. Phononic xy -displacement field of the screw dislocation (69), order $mn = 10$. Magnification of the displacement vectors: 6.

the displacements in Figure 10 refers to a $-\frac{4\pi}{5}$ -rotation of the vectors and a $\frac{2\pi}{5}$ -rotation of the positions.

The total correction of the displacement field has a z -component which is shown in Figure 11. Its tenfold symmetry is surprising, but it is the only way for the system to obey the constraint (66). The lowest orders having such a tenfold z -component in phonon space are $mn = 31$ and $mn = 40$, but the z -component of order $mn = 40$ is about 11 times as large as in order $mn = 31$, and provides the largest z -correction. The graph of Figure 11 is not exactly symmetric with respect to its extremal points.

The displacement fields exhibit no invariance under the action of an appropriate mirror plane containing the z -axis, as in case of the edge dislocation (68).

The eigenvalues of the stress tensor σ^u , which are constant in zeroth order, become clearly fivefold symmetric when taking into account higher orders. The main change

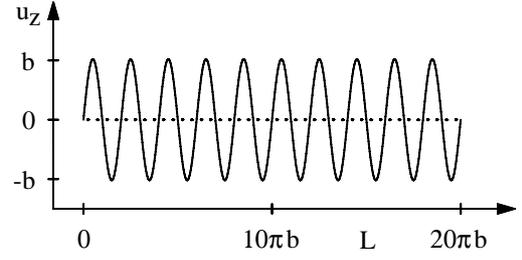


Fig. 11. Phononic z -displacement field of the screw dislocation (69), all orders mn with $m + n \leq 15$ except zeroth order. Magnification of the graph: 400 000.

away from isotropic behaviour is provided by orders mn where $m + n \leq 2$. Higher orders provide also a fivefold volume contraction, whereas in zeroth order there is none.

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Appendix A: Icosahedral irreducible strains

The icosahedral irreducible strains given here are taken from [12].

$$\varepsilon_1^u = \frac{1}{\sqrt{3}} (\varepsilon_{11}^u + \varepsilon_{22}^u + \varepsilon_{33}^u),$$

$$\varepsilon_5^u = \begin{bmatrix} \frac{1}{2\sqrt{3}} (-\tau^2 \varepsilon_{11}^u + \frac{1}{\tau^2} \varepsilon_{22}^u + (\tau + \frac{1}{\tau}) \varepsilon_{33}^u) \\ \frac{1}{2} (\frac{1}{\tau} \varepsilon_{11}^u - \tau \varepsilon_{22}^u + \varepsilon_{33}^u) \\ \sqrt{2} \varepsilon_{12}^u \\ \sqrt{2} \varepsilon_{23}^u \\ \sqrt{2} \varepsilon_{31}^u \end{bmatrix},$$

$$\varepsilon_4^w = \frac{1}{\sqrt{3}} \begin{bmatrix} \varepsilon_{11}^w + \varepsilon_{22}^w + \varepsilon_{33}^w \\ \frac{1}{\tau} \varepsilon_{21}^w + \tau \varepsilon_{12}^w \\ \frac{1}{\tau} \varepsilon_{32}^w + \tau \varepsilon_{23}^w \\ \frac{1}{\tau} \varepsilon_{13}^w + \tau \varepsilon_{31}^w \end{bmatrix}, \quad (\text{A.1})$$

$$\varepsilon_5^w = \frac{1}{\sqrt{6}} \begin{bmatrix} \sqrt{3} (\varepsilon_{11}^w - \varepsilon_{22}^w) \\ \varepsilon_{11}^w + \varepsilon_{22}^w - 2 \varepsilon_{33}^w \\ \sqrt{2} (\tau \varepsilon_{21}^w - \frac{1}{\tau} \varepsilon_{12}^w) \\ \sqrt{2} (\tau \varepsilon_{32}^w - \frac{1}{\tau} \varepsilon_{23}^w) \\ \sqrt{2} (\tau \varepsilon_{13}^w - \frac{1}{\tau} \varepsilon_{31}^w) \end{bmatrix}.$$

Appendix B: Elastic displacement fields of zeroth order

From (44, 61) and (62), the displacement field of zeroth order is

$$\begin{aligned} \gamma_{00} = & \frac{1}{2\pi} \left[b_x^u \left\{ \phi + \frac{(\lambda + \mu) xy}{(\lambda + 2\mu)(x^2 + y^2)} \right\} \right. \\ & + b_y^u \left\{ \frac{\mu}{\lambda + 2\mu} \ln \frac{r}{r_0} + \frac{(\lambda + \mu) y^2}{(\lambda + 2\mu)(x^2 + y^2)} \right\}, \\ & b_y^u \left\{ \phi - \frac{(\lambda + \mu) xy}{(\lambda + 2\mu)(x^2 + y^2)} \right\} \\ & - b_x^u \left\{ \frac{\mu}{\lambda + 2\mu} \ln \frac{r}{r_0} + \frac{(\lambda + \mu) x^2}{(\lambda + 2\mu)(x^2 + y^2)} \right\}, \\ & \left. b_x^u \phi, b_x^w \phi, b_y^w \phi, b_z^w \phi \right]^t. \end{aligned} \quad (\text{B.1})$$

Here, $\gamma_{00,1} = u_{00,x}, \dots, \gamma_{00,6} = w_{00,z}$. This displacement field is identical to the solution presented in [26] when $K_2 = 0$. $K_2 = 0$ corresponds to identical elastic constants $\mu_4 = \mu_5$, what is obvious from (C.1). The factor r_0 is introduced for dimensional reasons, and sometimes it is interpreted as inner cut-off for the linear elasticity [4].

The application of the projection method requires the knowledge of the solutions of the elastic equations of balance

$$\mathbf{D}_{00}(\nabla) \gamma''_\alpha + \delta(\mathbf{x}) \mathbf{f}''_{L\alpha} = \mathbf{0}, \quad (\text{B.2})$$

where the forces $\delta(\mathbf{x}) \mathbf{f}''_{L\alpha}$, $f''_{L\alpha,\beta} = \delta_{\alpha\beta}$, $\alpha, \beta = 1, \dots, 6$, represent point-like stress sources on the dislocation line (these prototypical forces are not body forces!). We have obtained the resulting fields using equation (23) with $\mathbf{G}_{00}(\mathbf{x} - \mathbf{x}')$. The γ''_α are

$$\begin{aligned} \gamma''_1 = & \frac{1}{4\pi} \left[-\frac{(\lambda + 3\mu)}{\mu(\lambda + 2\mu)} \ln \frac{r}{r_0} + \frac{(\lambda + \mu) x^2}{\mu(\lambda + 2\mu)(x^2 + y^2)}, \right. \\ & \left. \frac{(\lambda + \mu) xy}{\mu(\lambda + 2\mu)(x^2 + y^2)}, 0, 0, 0, 0 \right]^t, \\ \gamma''_2 = & \frac{1}{4\pi} \left[\frac{(\lambda + \mu) xy}{\mu(\lambda + 2\mu)(x^2 + y^2)}, -\frac{(\lambda + 3\mu)}{\mu(\lambda + 2\mu)} \ln \frac{r}{r_0} \right. \\ & \left. + \frac{(\lambda + \mu) y^2}{\mu(\lambda + 2\mu)(x^2 + y^2)}, 0, 0, 0, 0 \right]^t, \\ \gamma''_3 = & \frac{1}{2\pi} \left[0, 0, -\frac{1}{\mu} \ln \frac{r}{r_0}, 0, 0, 0 \right]^t, \\ \gamma''_4 = & \frac{1}{2\pi} \left[0, 0, 0, -\frac{1}{\mu_5} \ln \frac{r}{r_0}, 0, 0 \right]^t, \\ \gamma''_5 = & \frac{1}{2\pi} \left[0, 0, 0, 0, -\frac{1}{\mu_5} \ln \frac{r}{r_0}, 0 \right]^t, \\ \gamma''_6 = & \frac{1}{2\pi} \left[0, 0, 0, 0, 0, -\frac{1}{\mu_5} \ln \frac{r}{r_0} \right]^t. \end{aligned} \quad (\text{B.3})$$

These fields don't have the unit of a length, but our algorithm multiplies them by appropriate factors to become displacement fields.

Appendix C: Elastic constants

Different notations concerning the five independent elastic constants of icosahedral quasicrystals are in use.

To every elastic constant belongs a quadratic invariant of strain components. Different sets of elastic constants can be compared with each other, when the respective invariants are formulated in one and the same coordinate system. This can be achieved by means of coordinate transformations. Relations between different elastic constants arise from expressing one set of invariants by another and comparing the coefficients.

All authors we address also use the two Lamé-constants λ and μ (15), but a different phonon-phonon-coupling and other phasonic elastic constants.

In [11] and [26], the phonon-phason-coupling is denoted R , and the two phasonic elastic constants are K_1 and K_2 . The coordinate systems in phonon and phason spaces in these papers are transformed into our fivefold $K_5^{u,w}$ when substituting $x \rightarrow -x$, $y \rightarrow -y$, $z \rightarrow z$ and *vice versa*. Transforming our elastic tensor \mathbf{C}_5 in this manner allows a comparison with the parts \mathbf{R} and \mathbf{K} of the elastic tensor given explicitly in [11]. The relations between the elastic constants are

$$\begin{aligned} \mu_3 = \sqrt{6} R, & \quad R = \frac{1}{\sqrt{6}} \mu_3, \\ \mu_4 = K_1 - 2K_2, & \quad K_1 = \frac{1}{3}(\mu_4 + 2\mu_5), \\ \mu_5 = K_1 + K_2, & \quad K_2 = -\frac{1}{3}(\mu_4 - \mu_5). \end{aligned} \quad (\text{C.1})$$

The phonon-phason-coupling of [27] is denoted K_3 and the phasonic elastic constants are K_1 and K_2 , but with another meaning as in [11] and [26]. To compare the elastic energy expression of [27] with our equation (14), one must substitute ε_{ij}^w by ε_{ji}^w for all i, j . This is because the definition $\varepsilon_{ij}^w = \frac{\partial w_j}{\partial x_i}$ in [27] is different from our definition (8). In a second step, this new expression must be transformed into our coordinate systems of Figures 1, 2, what is achieved by subjecting all components $\varepsilon_{ij}^{u,w}$ to the coordinate transformation $x \rightarrow y$, $y \rightarrow -x$, $z \rightarrow z$. From the elastic energy density in this new form, we see that the elastic constants are related by

$$\begin{aligned} \mu_3 = -\sqrt{6} K_3, & \quad K_3 = -\frac{1}{\sqrt{6}} \mu_3, \\ \mu_4 = K_1 + \frac{5}{3} K_2, & \quad K_1 = \frac{1}{9}(4\mu_4 + 5\mu_5), \\ \mu_5 = K_1 - \frac{4}{3} K_2, & \quad K_2 = \frac{1}{3}(\mu_4 - \mu_5). \end{aligned} \quad (\text{C.2})$$

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