Physics Letters A 377 (2013) 2810–2814

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Elasticity and dislocations in quasicrystals with 18-fold symmetry

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ARTICLE INFO

Article history:
Received 28 April 2013
Received in revised form 4 July 2013
Accepted 20 August 2013
Available online 28 August 2013
Communicated by A.R. Bishop

Keywords:
Quasicrystal
Elasticity
Phason
Dislocation
18-fold symmetry
Constitutive equation

ABSTRACT

Elasticity problems of quasicrystals with 18-fold rotational symmetry are studied. Constitutive equations and governing equations are obtained. For static elasticity problems, the displacement vectors in two phason fields are expressed in terms of two pairs of associated harmonic functions or two analytic functions. For dynamic problems, the displacement vectors can be represented in terms of an auxiliary function satisfying a fourth-order partial differential equation. A general solution of phasons is given by the solution of two diffusion equations. Phason elastic fields induced by a dislocation in a quasicrystal with 18-fold symmetry are determined and exhibit an inverse singularity.

1. Introduction

Quasicrystals of icosahedral symmetry were observed in a rapidly cooled Al–Mn alloy for the first time in 1982 and reported in 1984 [1]. This discovery is one of the greatest discoveries in condensed matter and the discoverer, Shechtman, won the 2011 Nobel Prize in Chemistry for the discovery of quasicrystals. Conventional crystals only allow 2-, 3-, 4-, 6-fold rotational symmetries, and quasicrystals as an intermediate state between crystals and glassy solids possess quasiperiodic long-range translational symmetry and noncrystallographic rotational symmetry [2]. Up to now, quasicrystals with 5-, 8-, 10-, and 12-fold symmetry have been observed in experiment [1,3–5]. For these classes of quasicrystals, the research on their physical, mechanical, and electronic properties has attracted more and more attention of researchers. In particular, for quasicrystals as a new class of solids, their elasticity and deformation mechanism have been extensively studied from macroscopic continuum approach [6].

Quasicrystals may be understood as a projection of higher-dimensional periodic space [7]. Accordingly, differing from ordinary crystals possessing three displacement components as functions of three spacial coordinates, in quasicrystals, in addition to conventional three displacement components describing translations of particles, there are other displacement components which are used to describe rearrangements of local atomic configurations. Thus there are two typical subspaces, called parallel (physical, phonon) subspace and perpendicular (complementary, phason) subspace, respectively. Due to the presence of phasons, macroscopic properties of quasicrystals have apparent differences. For example, dislocations as typical topological defects are also in quasicrystals, but with nonvanishing phason's components accompanied with the Burgers vector of dislocations [8,9]. For quasicrystals with 5-, 8-, 10-, and 12-fold symmetry, elasticity theory has been established [10] and some typical solutions related to dislocations and cracks in the abovementioned quasicrystals have been solved by many researchers [11]. For instance, explicit expressions for the stress and displacement fields induced by a dislocation have been obtained with the aid of perturbation analysis method [12,13], Green's function [14,15], Fourier transform technique [16,17], and complex potential method [18–20], etc. Also, a static crack problem in quasicrystals has been tackled by various techniques (see e.g. [21,22]).

In the abovementioned researches, elasticity of quasicrystals only applies to quasicrystals with 5-, 8-, 10-, and 12-fold rotational symmetry. These quasicrystals contain one phonon field and one phason field. Recently, quasicrystals with 18-fold diffraction symmetry were observed in 2011 by Fischer et al. [23]. The latter differ from the former and must be embedded in a six-dimensional periodic space. Quasicrystals with 18-fold rotational symmetry embedded in a six-dimensional space were predicted in 1994 by Hu et al. [24], who studied the invariants of free elastic energy density as the quadratic form of all strains by the group representation theory. For such two-dimensional quasicrystals, in addition to a phonon field, two coupled phason fields are present. Consequently,

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0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.08.033

the elasticity theory applying to 5-, 8-, 10-, and 12-fold symmetric quasicrystals does not suit for 18-fold symmetric quasicrystals. There is little information on elastic analysis of 18-fold symmetric quasicrystals, to the best of the authors' knowledge.

This Letter considers elasticity of quasicrystals with 18-fold symmetry. First, constitutive equations or generalized Hooke's law describing stress–strain relationships are established. Furthermore, basic governing equations are given for static and dynamic problems. For static problems, the displacement vectors in two phason fields can be converted to two analytic functions, whereas for dynamic problems, a general solution of diffusion phasons is constructed. Finally, the stress fields induced by a dislocation in 18-fold symmetric quasicrystals are determined.

2. Basic equations

Consider a two-dimensional 18-fold symmetric quasicrystal which in the quasiperiodic plane can be understood as a projection of a six-dimensional periodic space. This class of two-dimensional quasicrystals are different from 5-fold quasicrystals. The latter only possesses a phason field, while the former has two coupled phason fields. Within the framework of continuum elasticity theory, three displacement vectors are present, one lying in the parallel subspace and two in the complementary subspaces denoted as $\mathbf{u} = (u_1, u_2, u_3)$, $\mathbf{v} = (v_1, v_2, v_3)$, $\mathbf{w} = (w_1, w_2, w_3)$, respectively. For convenience, in what follows the $\mathbf{v}$ and $\mathbf{w}$ phason fields are called the first and second phason fields, respectively. Since 18-fold symmetric quasicrystals are a two-dimensional quasiperiodic structure where the displacement vector in the quasiperiodic plane contain six components, two in the phonon field, two in the first phason field, and the remaining two in the second phason field. That is, $v_3 = w_3 = 0$. We take x_1 and x_2 as two mutual perpendicular axes in the quasiperiodic plane, and x_3 as the periodic axis. Using group representation theory, the energy density has been derived according to the quadratic invariants of all the strain components. In particular, for quasicrystals with 18-fold symmetry, the quadratic invariants of the energy density can be expressed as

$$\begin{aligned} U = {} & \frac{1}{2}\lambda(\nabla\cdot\mathbf{u})^2 + \mu\varepsilon_{ij}\varepsilon_{ij} + L_1^*\big[(v_{11}+v_{22})^2 + (v_{21}-v_{12})^2\big] \\ & + L_2^*\big[(v_{11}-v_{22})^2 + (v_{21}+v_{12})^2\big] \\ & + K_1^*\big[(w_{11}+w_{22})^2 + (w_{21}-w_{12})^2\big] \\ & + K_2^*\big[(w_{11}-w_{22})^2 + (w_{21}+w_{12})^2\big] \\ & + R_2\big[(v_{11}+v_{22})(w_{11}-w_{22}) + (v_{21}-v_{12})(w_{21}+w_{12})\big], \end{aligned} \tag{1}$$

where the summation convention on repeated indices has been used, λ and μ are the Lame constants, L_j^* and K_j^* $(j = 1, 2)$ represent positive elastic constants for two phason fields, R_2 is the phason–phason coupling constant; ε_{ij}, v_{ij} and w_{ij}, are defined by the displacements as follows, respectively

$$\varepsilon_{ij} = \frac{1}{2}(\partial_j u_i + \partial_i u_j), \tag{2}$$

$$v_{ij} = \partial_j v_i, \tag{3}$$

$$w_{ij} = \partial_j w_i, \tag{4}$$

where $\partial/\partial x_j$ is abbreviated as ∂_j. Consequently, in the x_1x_2-plane using

$$T_{ij} = \frac{\partial U}{\partial\varepsilon_{ij}}, \qquad Q_{ij} = \frac{\partial U}{\partial v_{ij}}, \qquad H_{ij} = \frac{\partial U}{\partial w_{ij}}, \tag{5}$$

one easily obtains the following constitutive equations of 18-fold symmetric quasicrystals in the quasiperiodic plane

$$T_{11} = (\lambda + 2\mu)\varepsilon_{11} + \lambda\varepsilon_{22}, \tag{6}$$

$$T_{22} = \lambda\varepsilon_{11} + (\lambda + 2\mu)\varepsilon_{22}, \tag{7}$$

$$T_{12} = 2\mu\varepsilon_{12}, \tag{8}$$

$$Q_{11} = L_1 v_{11} + L_2 v_{22} + R_2(w_{11} - w_{22}), \tag{9}$$

$$Q_{22} = L_2 v_{11} + L_1 v_{22} - R_2(w_{11} - w_{22}), \tag{10}$$

$$Q_{12} = L_1 v_{12} - L_2 v_{21} + R_2(w_{21} + w_{12}), \tag{11}$$

$$Q_{21} = -L_2 v_{12} + L_1 v_{21} + R_2(w_{21} + w_{12}), \tag{12}$$

$$H_{11} = K_1 w_{11} + K_2 w_{22} + R_2(v_{11} - v_{22}), \tag{13}$$

$$H_{22} = K_2 w_{11} + K_1 w_{22} - R_2(v_{11} - v_{22}), \tag{14}$$

$$H_{12} = K_1 w_{12} - K_2 w_{21} + R_2(v_{12} + v_{21}), \tag{15}$$

$$H_{21} = K_1 w_{21} - K_2 w_{12} + R_2(v_{12} + v_{21}), \tag{16}$$

where T_{ij}'s are phonon stress components, Q_{ij} and H_{ij} are phason stress components, which inhibit rearrangements of local atoms on a small scale and called as "pinning stresses". For convenience, we have used notations $L_1 = 2(L_1^* + L_2^*)$, $L_2 = 2(L_1^* - L_2^*)$, $K_1 = 2(K_1^* + K_2^*)$, $K_2 = 2(K_1^* - K_2^*)$. Obviously, λ, μ, L_1 and K_1 are positive, L_2 and K_2 may be positive and negative.

From the above definitions, one easily finds

$$\varepsilon_{ij} = \varepsilon_{ji}, \qquad v_{ij} \neq v_{ji}, \qquad w_{ij} \neq w_{ji}. \tag{17}$$

Furthermore, with the aid of constitutive equations, we find that the phonon stresses/strains are still symmetric tensor, but the phason stresses/strains are no longer symmetric tensor. That is,

$$T_{ij} = T_{ji}, \qquad Q_{ij} \neq Q_{ji}, \qquad H_{ij} \neq H_{ji}. \tag{18}$$

It is interesting to note that the basic equations of the phonon field are identical to those for ordinary crystals and they are uncoupled with the basic equations of two phason fields. As a result, the phonon field can be solved using the well-known elasticity theory for isotropic materials. Due to this reason, of much interest is elasticity problems related to the phason fields, which is new and does not appear for the classical elasticity theory.

Dynamic response of quasicrystals is a subject of considerable interest. Knowledge of dynamic response of phason in quasicrystals is very limited. A possible reason is that the physical mechanism of phase motion is not very clear. At the beginning of research of quasicrystals, phasons are usually assumed to obey Newton's second law in analogy to phonons [10],

$$\partial_j Q_{ij} = \rho_1\ddot{v}_i, \qquad \partial_j H_{ij} = \rho_2\ddot{w}_i, \tag{19}$$

where a dot denotes differentiation with respect to time t, ρ_1 and ρ_2 denote the effective phason mass density in the two perpendicular subspaces, respectively, which are different from ordinary mass density ρ in the parallel subspace. Here phason body forces are neglected. Now, due to some evidence observed in experiment, researchers prefer to assume that phasons exhibit diffusion characteristics [25,26], rather than to adopt propagating phasons, i.e.,

$$\partial_j Q_{ij} = \kappa_1\dot{v}_i, \qquad \partial_j H_{ij} = \kappa_2\dot{w}_i, \tag{20}$$

where κ_1 and κ_2 are material constants describing the damping or friction effect, which are the inverse of the dissipative kinetic coefficient Γ_v and Γ_w of the material. Furthermore, if diffusion and propagation characteristics are both taken into account, it is natural to consider the case where the phasons can propagate with damping. Thus we have

$$\partial_j Q_{ij} - \kappa_1\dot{v}_i = \rho_1\ddot{v}_i, \qquad \partial_j H_{ij} - \kappa_2\dot{w}_i = \rho_2\ddot{w}_i. \tag{21}$$