Dynamic coupling between phonon and phason dynamic modes in quasiperiodic alloys

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Abstract

The dynamic transfer of energy between phonon and phason modes in icosahedral quasicrystals is investigated, taking into account uncertainties in the value of phonon–phason coupling coefficient.

Keywords: Quasicrystals; Multifield theories; Random waves

1. Introduction

Analysis of X-ray diffraction patterns obtained from experiments on Al–Pb–Mn-based alloys has shown the existence of crystalline microstructures admitting icosahedral phase [1]. Bodies with such structures do not fit the rules summarized in the classification of crystallographic finite groups and for this reason are called quasicrystals (IQ). They are intrinsically quasiperiodic because lattices with icosahedral symmetry cannot fill the three-dimensional Euclidean space. Quasiperiodicity is assured by the presence of alterations of the crystalline lattice due to (i) collective atomic modes and (ii) tunneling of atoms below energetic barriers separating places at a distance less than the atomic diameter. Such substructural changes altering locally the material phase (thus referred to as phason activity) occur also in incommensurate intergrowth compounds (IIC), which are still quasiperiodic alloys but their quasiperiodicity is not intrinsic; rather, it is the result of modifications of originally periodic structures [2].

In modeling the mechanical behavior of IQ and IIC, it is not sufficient to describe the morphology of the material element only by means of its place in space as in standard elasticity, because geometrical information about substructural changes within the material element due to phason activity would be absent in this way. A morphological coarse-grained descriptor of the collective atomic modes within crystalline cells needs to be introduced by following the format of multifield theories [3,4] describing bodies with complex substructural morphology. In particular, to describe morphological changes in quasicrystals, two entities are necessary: the displacement field $\mathbf{u}$ and a vector field $\mathbf{w}$, which represents additional atomic (phason) modes within each crystalline cell. Interactions associated with phason changes (i.e. with the rate of $\mathbf{w}$) arise and are balanced appropriately. Their balance is additional to that of standard forces, which are power-conjugated only with deformation (phonon) modes.

In a dynamic regime, we may recognize waves of phonon and phason nature. Their interaction may be associated with a transfer of energy from microstructural to gross level, and vice versa. For IIC and IQ, the energetic landscape is different. In the diffraction scenarios obtained by X-ray scattering experiments, diffuse scattering is registered around Bragg peaks in both cases. However, for IIC there are six sound-like branches while in the case of IQ only three sound-like branches appear most often. As a consequence, kinetic energy can be attributed to the phason activity in the case of IIC, while for IQ there may be a type of internal friction leading to viscous-like evolution rather than true inertia effects. In other words, the collective atomic modes appearing in both IIC and IQ seem to have different natures; better, they develop in different physical circumstances [5,6]. Since in the case of IIC, at each point $\mathbf{X}$ the vector $\mathbf{w}$ represents the relative displacement of incommensurate sublattices, it is strictly a measure of deformation and does enter the structure of the free energy together with the gradient $\nabla\mathbf{w}$ of $\mathbf{w}$. It does not

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happen to IQ where only $\nabla\mathbf{w}$ appears in the list of constitutive entries of the energy. The partial derivatives of the energy with respect to $\mathbf{w}$ and $\nabla\mathbf{w}$ represent at thermodynamic equilibrium self-forces within the material element and phason stresses between neighboring material elements.

We follow a general (in a sense, unified) way to represent the mechanics of IIC and IQ [7,8] and restrict our attention to linear constitutive relations. We analyze different cases: (i) the presence of phason inertia, (ii) the presence of phason friction in absence of phason inertia, (iii) the contemporary presence of phason friction and inertia, and (iv) the absence of phason evolution (limit case).

In all of the above-listed circumstances, we analyze the spectral properties of the modified acoustic tensor accounting for phason modes. Such a tensor includes the coefficient of phonon–phason coupling. There is some experimental indeterminacy in the value of such a coefficient in linear constitutive equations. By taking into account such a circumstance, we analyze the spectral properties of the modified acoustic tensor as the phonon–phason coupling coefficients varies in a given range suggested by experiments. Our analysis allows to recognize conditions for which critical phenomena occur: they are associated with possible breaking and reconstruction of phonon and phason waves due to exchange of energy between material levels.

2. Elasticity for quasiperiodic alloys

A regular region B of the three-dimensional Euclidean point space $\mathcal{E}^3$ is occupied by a quasicrystalline body in its reference place. $\mathbf{X}$ indicates the generic point of it where a material element is *collapsed*. If we consider the material element as a perfect crystalline cell, then during a motion

$$B \times [0, \mathrm{t}^*] \ni (\mathbf{X},\ \mathrm{t}) \rightarrow \mathbf{x} = \mathbf{x}^*(\mathbf{X},\ \mathrm{t}) \in \mathcal{E}^3$$

developing in an interval of time [0,t*], the standard displacement field $\mathbf{u} = \mathbf{u}^*(\mathbf{X}, t) = \mathbf{x} - \mathbf{X}$ is the descriptor of the phonon degrees of freedom, i.e. of the standard waves.

In the case of quasiperiodic alloys, the material element is not a perfect cell because collective atomic modes and/or tunneling of atoms below energy barriers occur inside it and are represented by a sufficiently smooth vector field $\mathbf{w}^*$. During a motion, we then have:

$$B \times [0, \mathrm{t}^*] \ni (\mathbf{X},\ \mathrm{t}) \rightarrow \mathbf{w} = \mathbf{w}^*(\mathbf{X},\ \mathrm{t}) \in Vec$$

where Vec is the translation space over $\mathcal{E}^3$.

The dynamics of a quasicrystalline alloy are ruled by a Hamilton principle of the type

$$\delta \int_{B\times[0,\mathrm{t}^*]} \Big(0.5\Big(\rho\|\mathbf{x}^{\cdot}\|^2 + \rho^*\|\mathbf{w}^{\cdot}\|^2\Big) + e(\nabla\mathbf{u},\ \mathbf{w},\ \nabla\mathbf{w}) + \mathrm{U}(\mathbf{x})\Big)\, d\mathbf{X}^3 \wedge dt = 0$$

where $\mathrm{U}(\cdot)$ is the potential of possible external bulk forces, ρ the density of mass, and ρ^* an 'effective' density of mass associated with phonon modes, δ indicates variation and $e(\cdot)$ is the elastic energy.

Appropriate Euler–Lagrange equations are given by

$$\mathrm{Div}\mathbf{P} + \mathbf{b} = \rho\mathbf{x}^{\cdot\cdot} \quad \text{and} \quad \mathrm{Div}\mathbf{S} - \mathbf{z} = \rho^*\mathbf{w}^{\cdot\cdot}$$

where $\mathbf{P} = \partial_{\nabla\mathbf{u}} e$ is the first Piola–Kirchhoff stress, $\mathbf{S} = \partial_{\nabla\mathbf{w}}\, e$ the phason stress associated with contact interactions between neighboring material elements as a consequence of phason changes, $\mathbf{z} = \partial_{\mathrm{w}} e$ the self-force within each material element, and $\mathbf{b} = grad\mathrm{U}$ the vector of body forces.

In infinitesimal deformation regime, the first Piola–Kirchhoff stress $\mathbf{P}$ 'coincides' with Cauchy stress $\boldsymbol{\sigma}$, for IQ also $\mathbf{z}$ disappears and the constitutive equations take the form [9]

$$\boldsymbol{\sigma} = \mathbf{C}\nabla\mathbf{u} + \mathbf{K}'\nabla\mathbf{w}, \quad \mathbf{S} = \mathbf{K}'^T\nabla\mathbf{u} + \mathbf{K}\nabla\mathbf{w}$$

where the fourth-order tensors $\mathbf{C}$, $\mathbf{K}$, and $\mathbf{K}'$ are, respectively, the standard stiffness, the phason constitutive tensor, and the phonon–phason coupling constitutive tensor. For a two-dimensional quasicrystal with fivefold symmetry, $\mathbf{C}$ is the isotropic elastic tensor, and

$$\mathrm{K}_{\mathrm{ijkl}} = \mathrm{K}_1\, \delta_{\mathrm{ik}}\, \delta_{\mathrm{jl}} + \mathrm{K}_2(\delta_{\mathrm{ij}}\, \delta_{\mathrm{kl}} - \delta_{\mathrm{il}}\, \delta_{\mathrm{jk}}),$$
$$\mathrm{K}'_{\mathrm{ijkl}} = \mathrm{K}_3\, (\delta_{\mathrm{i1}} - \delta_{\mathrm{i2}})\, (\delta_{\mathrm{ij}}\, \delta_{\mathrm{kl}} - \delta_{\mathrm{ik}}\, \delta_{\mathrm{jl}} + \delta_{\mathrm{il}}\, \delta_{\mathrm{jk}})$$

depend on three real constants K_1, K_2 and K_3.

3. Interaction between phonon and phason modes

Planar waves in IQ satisfy the ansatz

$$\mathbf{u} = \mathbf{U}\exp[\mathrm{i}(\mathbf{k}\cdot\mathbf{x} - \omega t)] \qquad \mathbf{w} = \mathbf{W}\exp[\mathrm{i}(\mathbf{k}^{\mathrm{w}}\cdot\mathbf{x} - \Omega t)]$$

$\mathbf{U}$ and $\mathbf{W}$ denote the polarization of the phonon and phasonic waves, respectively, $\mathbf{k}$ and $\mathbf{k}^{\mathrm{w}}$ are the wave vectors, and ω and Ω are the cyclic frequencies. By substitution in the balance equations, in absence of body forces, we get

$$\begin{bmatrix} \mathbf{A}^u(\omega,\Omega) & \mathbf{0} \\ \mathbf{0} & \mathbf{A}^w(\omega,\Omega) \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{W} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{1}$$

where ω and Ω are eigenvalues. Matrices $\mathbf{A}^{\mathrm{u}}$ and $\mathbf{A}^{\mathrm{w}}$ depend on the four acoustic tensors

$\mathrm{B}^{\mathrm{u}}_{\mathrm{ik}} = \mathrm{C}_{\mathrm{ijkl}}\mathrm{k}_{\mathrm{l}}\mathrm{k}_{\mathrm{j}}$, $\quad \mathrm{B}^{\mathrm{w,coup}}_{\mathrm{ik}} = \mathrm{K}'_{\mathrm{ijkl}}\mathrm{k}^{\mathrm{w}}_{\mathrm{l}}\mathrm{k}^{\mathrm{w}}_{\mathrm{j}}$,
$\mathrm{B}^{\mathrm{u,coup}}_{\mathrm{ki}} = \mathrm{K}'_{\mathrm{klij}}\mathrm{k}_{\mathrm{l}}\mathrm{k}_{\mathrm{j}}$, $\quad \mathrm{B}^{\mathrm{w}}_{\mathrm{ik}} = \mathrm{K}_{\mathrm{ijkl}}\mathrm{k}^{\mathrm{w}}_{\mathrm{l}}\mathrm{k}^{\mathrm{w}}_{\mathrm{j}}$,

in the following way:

$$\mathbf{A}^u = (\mathbf{B}^{u,coup})^T + [\mathbf{B}^w - \rho^*\ \Omega^2\mathbf{I}]\ (\mathbf{B}^{w,coup})^{-1}[\rho\omega^2\mathbf{I} - \mathbf{B}^u],$$

$$\mathbf{A}^w = \mathbf{B}^{w,coup} + [\rho\omega^2\mathbf{I} - \mathbf{B}^u]\ (\mathbf{B}^{w,coup})^{-T}[\mathbf{B}^w - \rho^*\ \Omega^2\mathbf{I}]$$

Preliminary results are shown in Figs. 1, 2, and 3 for the case $\rho^* = 0$, relevant for IQ, and for specific values of K_1 and K_2. In this case, only the phonon frequency ω appears as an eigenvalue in Eq. (1). The components of the wave vectors for the three figures are given by $\mathbf{k} = (1,0)$ and $\mathbf{k}^w = (1, 0.1)$ (Fig. 1); $\mathbf{k} = (1,0)$ and $\mathbf{k}^w = (1, 1)$ (Fig. 2); and $\mathbf{k} = (1,0)$ and $\mathbf{k}^w = (1, 10)$ (Fig. 3). Plots of ω^2 [s^{-2}] versus the constant K_3 [Nm^{-2}] are depicted. It is shown that beyond a specific value of K_3 phonon waves cannot propagate.

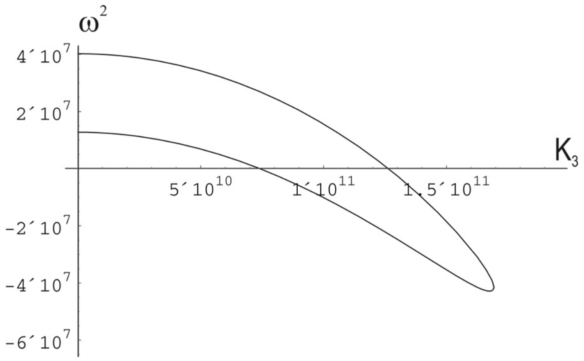

Fig. 1. Plot of ω^2 [s^{-2}] vs. the coupling modulus K_3 [Nm^{-2}] for IQ, for $\mathbf{k} = (1,0)$, $\mathbf{k}^w = (1,0.1)$.

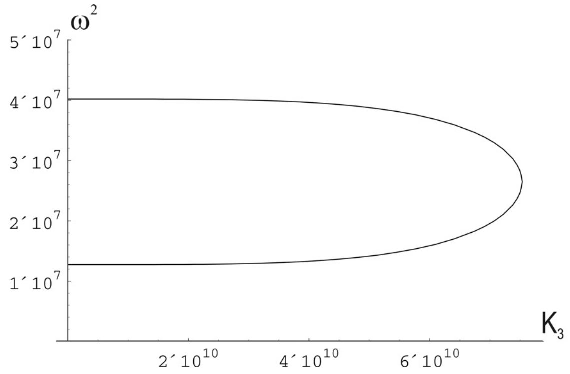

Fig. 2. Plot of ω^2 [s^{-2}] vs. the coupling modulus K_3 [Nm^{-2}] for IQ, for $\mathbf{k} = (1,0)$, $\mathbf{k}^w = (1,1)$.

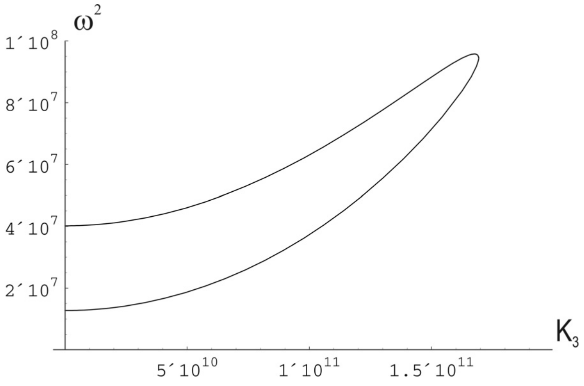

Fig. 3. Plot of ω^2 [s^{-2}] vs. the coupling modulus K_3 [Nm^{-2}] for IQ, for $\mathbf{k} = (1,0)$, $\mathbf{k}^w = (1,10)$.

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