Stochastic clustering and self-organisation of phonon and phason modes in quasicrystals

P.M. Mariano[a,*], F.L. Stazi[a], M. Gioffré[b], G. Augusti[a]

[a]*Dipartimento di Ingegneria Strutturale e Geotecnica, Università di Roma 'La Sapienza', Rome, Italy*
[b]*Dipartimento di Ingegneria Civile ed Ambientale, Università di Perugia, Perugia, Italy*

Abstract

Quasicrystals display random properties associated with the coupling coefficient between macroscopic (phonon) deformation and microstructural (phason) changes. With reference to the infinitesimal deformation regime, by coupling Monte Carlo simulation with finite element techniques, we show the possible existence of phenomena of stochastic clustering and self-organization of phonon and phason modes in icosahedral quasicrystals by considering the phonon–phason coupling coefficient as a random field over the body.

Keywords: Quasicrystals; Multifield theories; Random media

1. Introduction

Experiments developed using X-ray beams have shown that some metallic alloys display diffraction patterns with icosahedral symmetry, so that they are intrinsically quasiperiodic [1] because icosahedral structures alone cannot fill the space unless alterations of a different geometric nature are included. Such alterations induce quasiperiodicity. For this reason, such alloys are called *quasicrystals*. They were discovered in 1984 [2] and have since been used for energy savings and for the production of thin films, fillers for composites, and sinters.

To assure quasiperiodicity, substructural changes are allowed inside crystalline cells. They are (i) collective atomic modes and (ii) tunneling of atoms below energetic barriers at a distance less than the atomic diameter. Quasicrystals are, then, complex materials [3], and to represent the morphology of each material element one needs to introduce morphological descriptors of the substructural changes within each crystalline cell. In particular, the standard displacement field **u** is selected to represent common deformation (*phonon*) modes and a vector field **w** is used to describe additional atomic (*phason*) modes within each crystalline cell. We follow the mechanical description of quasiperiodic alloys in [4–6] and restrict the attention to the infinitesimal deformation regime. We consider the phonon–phason coupling coefficient as a random field over the body to capture uncertainties suggested by experiments in the evaluation of it. By means of Monte Carlo simulations coupled with finite element analyses, we evaluate the portraits of mean coefficient of variation, skewness, and kurtosis of phonon and phason modes in a four-point bending test and put in evidence phenomena of clustering and self-organization of phonon and phason modes. In this way, we extend the results given in [5].

2. Elasticity for quasiperiodic alloys

Let $\mathcal{B}$ be the regular (in the sense of 'fit') region of the Euclidean point space $\mathcal{E}^3$ occupied by a quasicrystalline body in its reference place. **X** is the generic point of it where a material element is *collapsed*. If we do not consider atomic changes within the material element, then during a motion:

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

'along' the 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 traveling waves. At each **X** and t, **u** is an element of the translation space Vec over $\mathcal{E}^3$.

* Corresponding author. Tel.: +39 06 44585276;
E-mail: paolo.mariano@uniroma1.it

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For quasicrystals, the material element is still a crystalline cell but is not perfect due to the presence of substructural changes as collective atomic modes and/or tunneling of atoms below energy barriers, which assure quasiperiodicity to atomic lattices. Internal changes accrue and are represented by a sufficiently smooth vector field $\mathbf{w}$. During a motion, we then have:

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

Notice that $\mathbf{u}$ and $\mathbf{w}$ belong strictly to different copies of *Vec*. In fact, the shift occurring in a material element collapsed in a place is of a different nature with respect to the macroscopic displacement of the material element itself described by $\mathbf{u}$.

In the case of elastic quasicrystals, the elastic energy displays a constitutive structure of the form $e = e^*(\nabla\mathbf{u}, \nabla\mathbf{w})$, so that the total energy of the body is given in referential representation by:

$$\int_{\mathcal{B}} (e^*(\nabla\mathbf{u}, \nabla\mathbf{w}) + \mathrm{U}(\mathbf{x}))\ \mathrm{d(vol)}$$

where $\mathrm{U}(\cdot)$ is the potential of possible external bulk forces.

At equilibrium, under suitable conditions of smoothness for $e^*(\cdot,\cdot)$ and $\mathrm{U}(\cdot)$, appropriate Euler–Lagrange equations are given by:

$$\mathrm{Div}\ \mathbf{P} + \mathbf{b} = \mathbf{0} \text{ and } \mathrm{Div}\ \mathbf{S} = \mathbf{0}$$

where $\mathbf{P} = \partial_{\nabla\mathbf{u}} e$ is the first Piola–Kirchhoff stress, $\mathbf{S} = \partial_{\nabla\mathbf{w}} e$ is the phason stress associated with substructural changes within each crystalline cell, and $\mathbf{b} = grad\mathrm{U}$ is the vector of body forces, with *grad* the gradient with respect to $\mathbf{x}$. The phason stress indicates contact interactions between neighboring material elements as a consequence of phason changes within at least one of them.

Invariance of $e^*(.,.)$ under rotations of observers implies also

$$\mathbf{e}(\mathbf{P}\mathbf{F}^{\mathrm{T}} - (\nabla\mathbf{w})^{\mathrm{T}}\mathbf{S}) = \mathbf{0}$$

with $\mathbf{e}$ being Ricci's alternator index and $\mathbf{F} = \nabla\mathbf{x}$ being the standard deformation gradient. If we restrict our treatment to the infinitesimal deformation regime in which $\mathbf{P} \approx \boldsymbol{\sigma}$ and $\mathbf{S} \approx \mathbf{S}_{\mathrm{a}}$, where σ is Cauchy's stress and $\mathbf{S}_{\mathrm{a}}$ is the phason stress in the current place, and consider a linear constitutive behavior, we get:

$$\mathbf{P} \approx \boldsymbol{\sigma} = \mathbf{C}\nabla\mathbf{u} + \mathbf{K}'\nabla\mathbf{w}, \mathbf{S} \approx \mathbf{S}_{\mathrm{a}} = \mathbf{K}'\nabla\mathbf{u} + \mathbf{K}\nabla\mathbf{w}$$

In this case, the elastic energy is the sum of three contributions: (i) a pure phonon part $0.5\mathbf{C}\nabla\mathbf{u}\cdot\nabla\mathbf{u}$, (ii) a pure phason part $0.5\ \mathbf{K}\nabla\mathbf{w}\cdot\nabla\mathbf{w}$, and (iii) an interaction energy $\mathbf{K}'\nabla\mathbf{w}\cdot\nabla\mathbf{w}$. In the case of a *planar quasicrystal with fivefold symmetry*, we get:

$$\mathrm{C}_{\mathrm{ijkl}} = \lambda\delta_{\mathrm{ij}}\delta_{\mathrm{kl}} + \mu(\delta_{\mathrm{ik}}\delta_{\mathrm{jl}} + \delta_{\mathrm{il}}\delta_{\mathrm{jk}})$$

i.e. the standard expression for simple isotropic elastic bodies where λ and μ are the Lamè constants, δ_{ij} is the Kroenecker delta, and

$$K_{\mathrm{ijkl}} = K_1\delta_{\mathrm{ik}}\delta_{\mathrm{jl}} + K_2(\delta_{\mathrm{ij}}\delta_{\mathrm{kl}} + \delta_{\mathrm{il}}\delta_{\mathrm{jk}})$$
$$K'_{\mathrm{ijkl}} = R(\delta_{\mathrm{il}} - \delta_{\mathrm{j2}})(\delta_{\mathrm{ij}}\delta_{\mathrm{kl}} - \delta_{\mathrm{ik}}\delta_{\mathrm{jl}} + \delta_{\mathrm{il}}\delta_{\mathrm{jk}})$$

where no summation is assumed on repeated indices.

3. Interaction between phonon and phason modes

The way in which one may estimate the phonon–phason coupling coefficient R is not well established. Theoretical models suggest R to be of at least one order of magnitude smaller than K_1 and K_2. However, experiments based on X-ray diffuse scattering in a grain of Al–Pb–Mn quasicrystals indicate a value of R larger than K_1 and K_2, at least for samples in which off-stoichiometry defects are included in a single phase. In some circumstances, X-ray diffuse scattering data would suggest that R vanishes, but such an interpretation appears unrealistic: the elastic distortion influences phason activity because it changes the energetic content of each crystalline cell. Due to experimental uncertainties, the phonon–phason coupling coefficient R is considered here as varying at random over the body (thus as a stochastic field over $\mathcal{B}$) because quasicrystals may be pictured by means of random tessellation (e.g. Penrose tiling) of the space they occupy.

As a sample case, we consider R as a homogeneous stochastic field over $\mathcal{B}$ described by a *beta distribution* between $R = 0.01K_1$ (a value at which it is practically impossible to evaluate experimentally the velocity anisotropy between modes propagating along fivefold axis and modes along twofold axis) and $R = K_1$; moreover, we select $\lambda = 0.75\times10^{11}$ N/m^2 $\mu = 0.65 \times 10^{11}$ N/m^2, $K_1 = 0.81 \times 10^{11}$ N/m^2, and $k_2 = -0.42 \times 10^{11}$ N/m^2, while the parameters in the beta distribution are set at $r = 73.5455$, $s = 735.4545$, so that the mean value of R is $0.1K_1$. By connecting finite elements with Monte Carlo simulations, we evaluate the relevant statistics of the phonon and phason displacements in a rectangular sample endowed with a crack and submitted to a four-point bending test (Fig. 1) under forces each equal to 10 N.

The results show the existence of patterns suggesting self-organization and clustering of phonon and phason modes, a result not recognized so far. These patterns depend on the stochastic spatial correlation of data: the larger effects occur in case of perfect correlation, and the smaller is obtained in absence of correlation. The results associated with the case of perfect correlation (called,

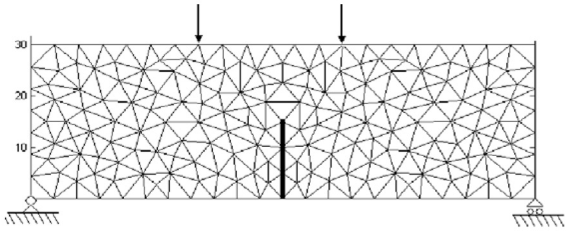

Fig. 1. Fourpoints bending test. X-axis: horizontal. Y-axis: vertical.

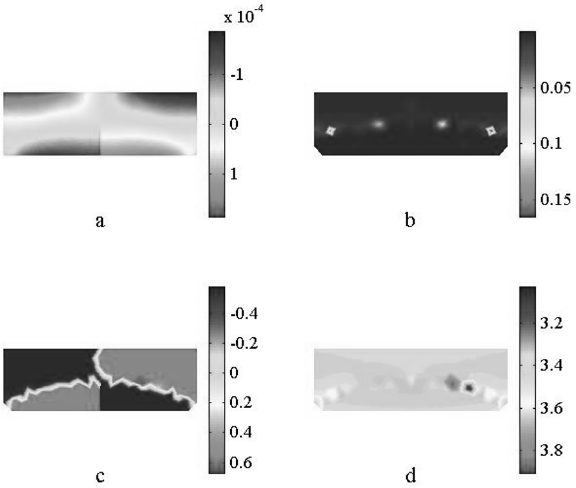

Fig. 2. Phonon modes along x-axis: case H: (a) mean; (b) coefficient of variation; (c) skewness; (d) kurtosis.

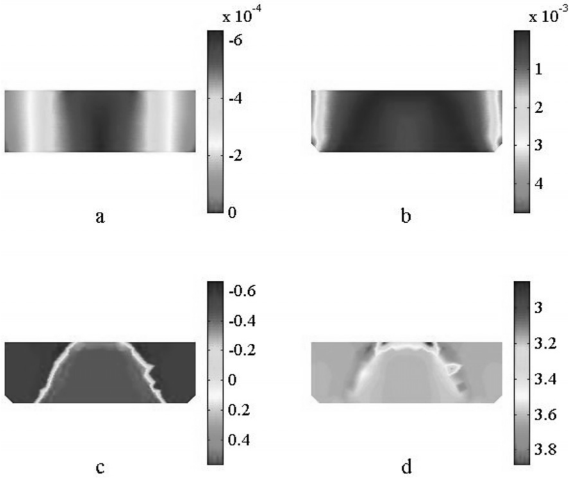

Fig. 3. Phason modes along x-axis: case H: (a) mean; (b) coefficient of variation; (c) skewness; (d) kurtosis.

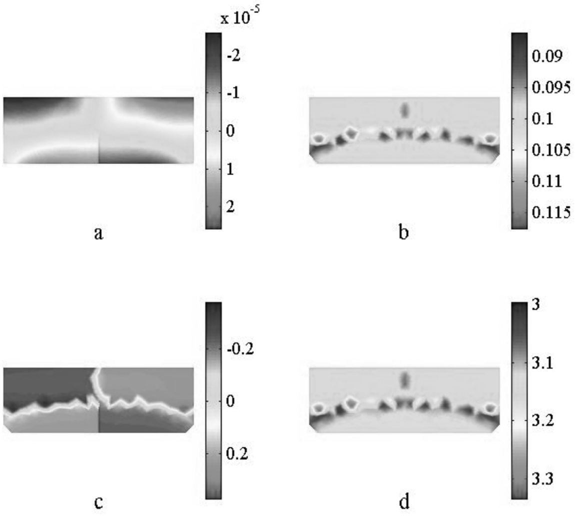

Fig. 4. Phonon modes along y-axis: case H: (a) mean; (b) coefficient of variation; (c) skewness; (d) kurtosis.

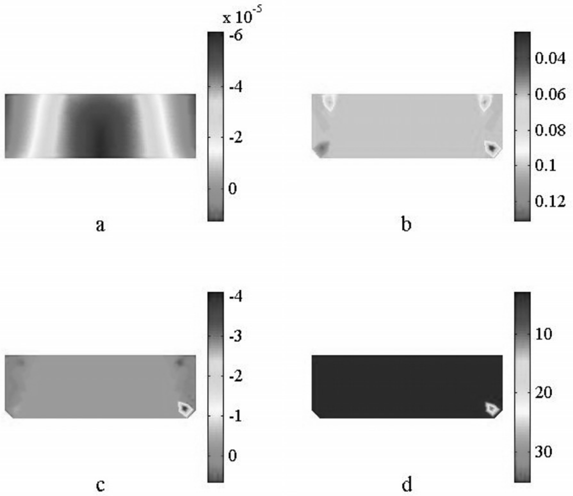

Fig. 5. Phason modes along y-axis: case H: (a) mean; (b) coefficient of variation; (c) skewness; (d) kurtosis.

here, 'case H') are presented in Figs 2–5. Of course, the case of perfect correlation must be interpreted just as upper bound.

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