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Mechanics of Quasi-Periodic Alloys

P. M. Mariano

Dipartimento di Ingegneria Strutturale e Geotecnica, Università di Roma "La Sapienza," via Eudossiana 18, I-00184 Roma, Italy e-mail: paolo.mariano@uniroma1.it

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Summary. A general description of the nonlinear mechanical behavior of quasi-periodic alloys is presented: It accounts for the rearrangements of atomic clusters (phason activity) and is based on a Lagrange-d'Alambert-type principle where phason dissipative effects are included. We find the covariance of the balance of phason interactions in the presence of phason friction, discuss the formulation of appropriate conservative and dissipative brackets, and recognize for quasicrystals the universality of affine deformations and affine phason activity at equilibrium for vanishing phason friction. Moreover, we investigate the nature of the influence of phason activity on a macroscopic discontinuity surface endowed with its own surface energy and find covariant interface balances describing its evolution. Finally, we investigate the nature of the balance of phason interactions in the bulk material and relate it to SO(3) invariance.

Key words. quasi-periodic alloys, interfaces, multifield theories

1. Introduction

A standard crystalline lattice is a \mathbb{Z} -module over the ambient space, characterized by periodicity and symmetries described by the crystallographic groups. However, experiments based on X-ray scattering techniques display the existence of alloys for which periodicity, i.e., translational symmetry, is violated, but not as a common consequence of the presence of defects. These alloys are constituted by *quasi-periodic* crystalline lattices that we may roughly divide in three classes (see [36]) analyzed in the subsequent sections.

(i) We may imagine first a perfectly periodic structure, a standard crystalline lattice. We "modulate" it by "displacing" ideal locations of atoms in a manner in which the original period of the translational symmetry is incommensurate with respect to the "period" of the modulation. Alloys with this nature are called *incommensurate modulated crystals* (IMC).

- (ii) Another family of quasiperiodic structures is the one of *incommensurate inter-growth compounds (composite crystals)* (IIC) characterized by the presence of two or more (sub)lattices with periods mutually incommensurate. These sublattices shift reciprocally to try to match one another. Moreover, a more complicated landscape may occur when each sublattice is not a standard crystalline lattice but is itself an incommensurate modulated structure.
- (iii) Both IIC and IMC are obtained by starting from standard crystalline lattices (by superposition or modulation) and are in this sense exotic offsprings of the standard crystallographic realm. In 1984, Shechtman and co-workers [37] discovered the existence of intrinsically quasi-periodic structures, the so-called *quasicrystals*, that satisfy symmetries forbidden by the classification of crystallographic groups [21]: icosahedral symmetry in space and pentagonal symmetry in the plane, for example. They may display five-fold, eight-fold, ten-fold symmetries. To have a clear idea, let us think of a planar ambient space and try to construct over it a lattice with pentagonal symmetry covering the whole plane. From elementary geometry we know that we cannot fill the plane by using only pentagons, so that we are forced to insert here and there topological alterations (i.e., structures different from pentagons) called "worms," that alter periodicity. Worms also appear to be necessary in three-dimensional space when one would try to construct a lattice with an icosahedral modulus [37]. A suggestive portrait of quasicrystals is given by Penrose tiling (see [32]).

Substructural events occur in quasi-periodic alloys within each crystalline cell: They are local rearrangements of atomic clusters and influence the gross mechanical behavior because they change the global energetic landscape in a nonnegligible manner. To describe the substructural interactions generated by energetic variations at atomic scale, we follow the general format of multifield theories for complex bodies [5], [24], and assign to each material element a morphological descriptor of the substructural changes *within* the element itself, changes that are referred to as *phason activity*. In this way we follow a common practice in which the word "phason" is used to indicate modes that alter locally the crystalline phase in addition to global acoustic ("phonon") modes generated by the gross deformative behavior.

For the substructural events occurring in quasi-periodic alloys, a natural descriptor is a vector **w** attached at each point. In the case of IIC and IMC, it represents a true microdisplacement, the one necessary to modulate an original periodic structure in IMC or the one describing the shift between sublattices in IIC. In the case of quasicrystals the interpretation is more subtle. In fact, if one develops in Fourier series the mass density ρ (**x**) on a three-dimensional quasi-crystalline lattice with icosahedral symmetry, the Fourier amplitude is given by $|\rho_k| \exp i \Phi_k$ with $\Phi_k = \Phi_{k,0} + \mathbf{k} \cdot \mathbf{u} + \mathbf{k'} \cdot \mathbf{w}$, where **u** and **w** are three-dimensional vectors (representing phonon and phason degrees of freedom respectively), $\Phi_{k,0}$ is the value of Φ_k at a ground state. As a consequence, we cannot represent in Fourier series the mass density over a three-dimensional quasi-periodic lattice by using only one wave vector in \mathbb{R}^3 ; we are forced to work in a high-dimensional

(here six-dimensional) space. In this sense a quasi-crystalline lattice can be considered as the projection in the three-dimensional space of a high-dimensional periodic lattice [11]. Vice versa, we might imagine embedding three-dimensional quasi-crystalline lattices in a high-dimensional space and utilizing in that space the standard crystallographic classification techniques. In this way an indeterminacy accrues because the embedding is not unique, so that it would appear convenient to treat everything in Fourier space as suggested in [35]. However, by means of appropriate gauge functions, it is possible to link Fourier representation with high-dimensional "ambient" space representation, eliminating the indeterminacy [12], [19] (see also [18] for related matter).

Phason activity develops in quasicrystals: It is constituted by collective atomic modes and/or tunneling of atoms below energetic barriers separating neighboring places [9], [34]: They "perturb" standard phonon elastic modes so that, for us, the vector **w** represents locally such an influence.

The three classes of quasi-periodic alloys listed in the items (i)–(iii) display different energetic landscapes.

- (a) IIC and IMC may admit phason kinetics, while, in contrast, in quasicrystals phason inertia is absent: X-ray-based experiments show, in fact, that only three acoustic modes (the ones associated with standard translational degrees of freedom in the ambient space) are present in scattering spectra. In IIC and IMC, structural defects may generate a "pinning" effect that bars phason inertia.
- (b) For IIC and IMC, the internal energy depends not only on the macroscopic measures of deformation but also on the morphological descriptor **w** of the phason activity and its spatial gradient ∇ **w**. The dependence on **w** is justified by the circumstance that **w** represents a *relative* displacement in IIC and IMC, in a certain sense a sort of measure of deformation *within* each crystalline cell. In contrast, in the case of quasicrystals, the elastic energy depends on ∇ **w** and not on **w**. In particular, the dependence on ∇ **w** is quadratic in the so-called "unlocked" phase while it is just on the modulus of ∇ **w** in the so-called "locked" phase where "phasons cannot be thermodynamically excited" [18].
- (c) Phason friction occurs in general in quasicrystals (it vanishes of course at zero Kelvin). Moreover, phason friction may or may not be recognized in IIC and IMC, depending on circumstances, but independently of the presence (or absence) of phason inertia.

The mechanics of quasi-crystalline alloys has been discussed variously in scientific literature, above all with reference to quasicrystals (see, e.g., [8], [11], [18], [22], [33], [34]). Primarily, the attention has been focused on some aspects of infinitesimal strain regime and on the possible nature of constitutive laws in nonlinear elastic behavior, neglecting phason friction (see [33]).

Here we tackle the matter from a general point of view. The outline of this paper is summarized below:

• A general formulation of the mechanics of IIC, IMC, and quasicrystals is presented here. It is based on a variational principle of Lagrange-d'Alambert type that accounts for dissipative effects due to phason friction.

- A Noether-like theorem is proven (Theorem 1): Its main peculiarity is that it accounts for phason friction. The result is nonstandard because the Noether theorem is commonly derived in a conservative setting.
- Theorem 1 implies a number of corollaries. The covariance of the balances of phonon and phason interactions follow first. Here, "covariance" means invariance with respect to changes in observers differing by transformations belonging to groups larger than *SO* (3) (i.e., the one associated with standard rigid body motions) and including it. The covariance of the balance of phonon interactions (common bulk forces and stresses) is a standard result in nonlinear elasticity (see [29]). That the balance of phason interactions, including phason friction, is also covariant is a new result (Corollary 1). Moreover, the presence of phason interactions renders nonsymmetric Cauchy stresses (Corollary 2) as a consequence of *SO* (3) invariance.
- The requirement of invariance of the Lagrangian density with respect to the relabeling of the reference place (i.e., the invariance with respect to the "permutation" of possible defects) allows us to derive from Theorem 1 a balance of "configurational" forces accounting for phason effects (friction included) that is invariant under the action of the special group of isochoric diffeomorphisms (Corollary 3). An extended Eshelby stress is involved: It satisfies an appropriate Doyle-Ericksen-like formula (Theorem 3), while for Cauchy stress the traditional Doyle-Ericksen formula is modified by the contribution of the phason (micro)stress (formula (69)).
- Affine bulk deformations and affine phason activity constitute a class of universal solutions to the equilibrium problem of quasicrystals in a nonlinear elastic setting, in the theoretical limit of vanishing phason friction (Theorem 2). In contrast to the standard case of nonlinear elasticity of simple bodies, here it is necessary that the derivatives of the stress measures (first Piola-Kirchhoff stress tensor and referential microstress) satisfy an algebraic pointwise condition.
- Poisson brackets for IIC and IMC in pinning free states are introduced in Section 4 for the pure elastic case when phason friction is absent. They allow one to represent concisely the field equations (Theorem 4), to point out that the algebra of smooth functions over the phase space (some of such functions are candidates to be Hamiltonians) is endowed with Lie structure, to open the way to a class of numerical schemes. Dissipative brackets accounting for phason friction are presented in Section 5.
- Linearization of the nonlinear theory presented in this paper is briefly discussed in Section 6: Existing linear theories on the mechanical behavior of quasi-periodic alloys are special cases. Unaspected results on wave propagation in *AlPbMn*-based alloys, obtained in the linearized setting, are also summarized in the same section.
- There are circumstances in which wall defects are present in quasi-periodic alloys and evolve relative to the body itself. They are represented in this paper by means of surfaces where some fields suffer bounded discontinuities: Their evolution is influenced by phason activity, as shown in Section 7. We focus attention on a single discontinuity surface, consider it coherent and anisotropic, and assume also that it is structured in the sense that it may sustain standard and phason surface stresses, also a surface self-force. We derive an evolution equation by exploiting the action of the special group of isochoric diffeomorphisms that relabel points on the discontinuity surface. Such an evolution is a generalization of the motion-by-curvature and accounts for

both macroscopic deformations and phason activity. Interface balances of standard (phonon) and phason interactions are also derived in a covariant way (Theorem 5).

• The covariance of all balance equations obtained below suggests that they are more fundamental (in a certain sense, more universal) in the physics we are considering than suggested by the standard requirement of invariance with respect to changes in observers governed by rigid body motions (ruled by *SO*(3)). However, *SO*(3) invariance allows one to get a nontrivial interpretation of global integral balances and the pointwise balance of phonon interactions in the bulk. The latter balance follows, in fact, by requiring that the external power of all actions over any arbitrary part (with nonvanishing volume) of the body be *SO*(3) invariant. In doing calculations, in fact, we find the existence of an internal self-force of phason nature independently of constitutive assumptions, a self-force that is commonly postulated. The structure of such a self-force is then specified by constitutive laws, namely for quasicrystals it has only dissipative nature, while for IIC and IMC it also admits a conservative part.

Some notations. For any pair of vector spaces A and B (with duals A^* and B^*), Hom (A, B) is the space of linear maps from A to B. For any manifold M, $T_m M$ is the tangent space of M at $m \in M$, while T_m^*M is the relevant cotangent space. Moreover, Aut (A) indicates the space of automorphisms of A. By the letters \mathcal{B}_0 and \mathcal{B} we will indicate two different regular bounded regions of the three-dimensional Euclidean point space \mathcal{E}^3 , and by \mathbb{V}_u and \mathbb{V}_w two different copies of the translation space of \mathcal{E}^3 (we may also identify them as copies of \mathbb{R}^3). Capital letters A, B, C... used as indices denote coordinates in \mathcal{B}_0 , while *i*, *j*, *k*... denote coordinates in \mathcal{B} . The differential operators *Div* and ∇ indicate respectively divergence and gradient calculated with respect to coordinates in \mathcal{B}_0 , while *div* and *grad* are their counterparts with respect to coordinates in \mathcal{B} . The superscript T means transposition. The symbol ∂_{y} means partial derivative with respect to the entry "y." We indicate by the term *part* any subset of \mathcal{B}_0 with nonvanishing volume and the same regularity properties of \mathcal{B}_0 . Let Σ be any smooth surface in \mathcal{B}_0 oriented by the normal **m** at each point, for any field $e(\cdot)$ defined on \mathcal{B}_0 and differentiable there; we indicate by ∇_{Σ} its surface gradient along Σ , namely, $\nabla_{\Sigma} e(\mathbf{X}) = \nabla e(\mathbf{X}) (\mathbf{I} - \mathbf{m} \otimes \mathbf{m})$, with I the second-order unit tensor. The trace of $\nabla_{\Sigma} e$ is the surface divergence of e, namely, $Div_{\Sigma} e$. Other notations will be explained later.

2. Configurations, Observers, and Relabeling

2.1. Configurations

A quasi-periodic crystalline body occupies in its reference place a fit region \mathcal{B}_0 of the three-dimensional Euclidean point space \mathcal{E}^3 . A generic point $\mathbf{X} \in \mathcal{B}_0$ is identified with the centre of mass of a crystalline cell (which is the *characteristic material element*) that one may imagine collapsed at \mathbf{X} in a coarse-grained representation of the quasi-periodic structure.

A *standard deformation* of the body is given by such a sufficiently smooth injective mapping $\mathcal{B}_0 \ni \mathbf{X} \xrightarrow{\tilde{\mathbf{x}}} \mathbf{x} = \tilde{\mathbf{x}} (\mathbf{X}) \in \mathcal{E}^3$ that the current place $\mathcal{B} = \tilde{\mathbf{x}} (\mathcal{B}_0)$ of the body is a regular region too. The *placement map* $\tilde{\mathbf{x}}$ is also orientation-preserving: at each \mathbf{X} its

gradient $\mathbf{F} = \nabla \mathbf{x}$ has positive determinant. \mathbf{F} is the value of the map $\mathcal{B}_0 \ni \mathbf{X} \xrightarrow{\tilde{\mathbf{F}}} \mathbf{F} = \tilde{\mathbf{F}}(\mathbf{X}) \in Hom(T_{\mathbf{X}}\mathcal{B}_0, T_{\mathbf{x}}\mathcal{B}).$

Let **g** be the spatial metric in \mathcal{B} and γ be the material metric in \mathcal{B}_0 . The linear operator $\mathbf{F}^T \mathbf{F} = \mathbf{C} \in Hom(T_{\mathbf{X}}\mathcal{B}_0, T_{\mathbf{X}}^*\mathcal{B}_0)$ is the pull-back at **X** of **g** through $\tilde{\mathbf{x}}$, i.e., in coordinates, $C_{AB} = F_A^{Ti} g_{ij} F_B^j$. Then, the difference $(\mathbf{C} - \gamma)$ is twice the nonlinear deformation tensor **E**.

If we consider each material element as a perfect crystalline cell, during a motion $\mathcal{B}_0 \times [0, \tilde{t}] \ni (\mathbf{X}, t) \stackrel{\tilde{\mathbf{x}}}{\mapsto} \mathbf{x} = \tilde{\mathbf{x}} (\mathbf{X}, t) \in \mathcal{E}^3$, the standard displacement field $\mathbf{u} = \tilde{\mathbf{u}} (\mathbf{X}, t) = \tilde{\mathbf{x}} (\mathbf{X}, t) - \mathbf{X} \in \mathbb{V}_u$ is the descriptor of *phonon degrees of freedom* (the ones associated with ordinary acoustic regime). \mathbb{V}_u is a copy of the translation space \mathbb{V} over \mathcal{E}^3 and can be identified with \mathbb{R}^3 .

In standard periodic crystals, the displacement field is the sole basic kinematical descriptor of the gross behavior. When the crystalline structure is quasi-periodic, substructural events at the atomic scale occur "within" each material element and are of various natures. To represent their effects at coarse scale, we attach at each point a morphological descriptor of what happens "inside" the material element, and we find it convenient to identify it with a three-dimensional vector **w** carrying information about local rearrangements of the crystalline structure, the so-called *phason degrees of freedom*. A vector field $\mathcal{B}_0 \ni \mathbf{X} \stackrel{\tilde{\mathbf{w}}}{\longrightarrow} \mathbf{w} = \tilde{\mathbf{w}}(\mathbf{X}) \in \mathbb{V}_w$ is then defined, and we presume that it is sufficiently smooth. During a motion, we get $\mathcal{B}_0 \times [0, \bar{t}] \ni (\mathbf{X}, t) \stackrel{\tilde{\mathbf{w}}}{\longmapsto} \mathbf{w} = \tilde{\mathbf{w}}(\mathbf{X}, t) \in \mathbb{V}_w$, with a slight abuse of notation.

From the point of view of the general setting of *multifield theories*, the copy \mathbb{V}_w of the translation space \mathbb{V} over \mathcal{E}^3 , containing ws, plays the role of a *manifold of substructural shapes* [5], [24].

Of course, the physical meaning of w changes according to the situation envisaged.

- (i) In the case of *incommensurate intergrowth compounds* (IIC), **w** represents the *shift* between mutually incommensurate lattices that occurs under mechanical loading.
- (ii) For *incommensurately modulated crystals* (IMC), w represents the microdisplacement needed locally to break the three-dimensional translation symmetry of the original periodic structure to obtain the quasi-periodic (modulated) one.
- (iii) For *quasicrystals*, w is a coarse-grained representative of the effects of substructural rearrangements in the crystalline patches, such as relocation of atoms [18], due to jumps of the atoms "from one position to another one nearby having a similar local environment" [9], or collective atomic modes generated for example by the flipping of crisscrossing worms needed to maintain matching rules [17].

In the case of incommensurate intergrowth compounds, since **w** represents a real local microdisplacement, a global displacement $\bar{\mathbf{u}}$ belonging to $\mathbb{V}_u \oplus \mathbb{V}_w$ can be considered in principle. A similar choice is also rather natural for IMC and is proposed even in the case of quasicrystals (see [8], [17]).

By indicating by $\mathbf{x}' = \tilde{\mathbf{x}}'(\mathbf{X})$ the point given by $\mathbf{x}' = \mathbf{X} + \bar{\mathbf{u}} = \mathbf{X} + \bar{\mathbf{u}} + \mathbf{w}$, and by \mathbf{F}' the gradient $\nabla \tilde{\mathbf{x}}'(\mathbf{X})$, we get additive and multiplicative decompositions given respectively by $\mathbf{F}' = \mathbf{F} + \nabla \mathbf{w}$ and $\mathbf{F}' = \mathbf{F}^{ph}\mathbf{F}$, with $\mathbf{F}^{ph} = \mathbf{I} + (\nabla \mathbf{w})\mathbf{F}^{-1}$. Really, since $\tilde{\mathbf{x}}$ is one-to-one, one may construct a representation of \mathbf{w} on the "apparent" current place

 \mathcal{B} of the body. By indicating by $\mathbf{w}_a = \tilde{\mathbf{w}}_a(\mathbf{x})$ the image of \mathbf{w} attached at $\mathbf{x} = \tilde{\mathbf{x}}(\mathbf{X}) \in \mathcal{B}$, we get $\tilde{\mathbf{w}}_a = \tilde{\mathbf{w}} \circ \tilde{\mathbf{x}}^{-1}$ so that $(\nabla \mathbf{w}) \mathbf{F}^{-1} = \operatorname{grad} \mathbf{w}_a$. As a consequence, the interpretation of the multiplicative decomposition of \mathbf{F} may be the following: Ideally, in the case of IIC we may deform first the body at a coarse-grained level, then we may allow the sublattices to slip with one another. In other words, by indicating by $\tilde{\mathbf{x}}^{ph}$ the mapping $\tilde{\mathbf{x}}^{ph} = \tilde{\mathbf{x}}' \circ \tilde{\mathbf{x}}^{-1}$, we realize that $\mathbf{F}^{ph} = \mathbf{I} + \operatorname{grad} \mathbf{w}_a$ is the gradient of deformation from \mathcal{B} to $\tilde{\mathbf{x}}^{ph}$ (\mathcal{B}), and there is such a map $\tilde{\mathbf{F}}^{ph}$ (considered here to be piecewise continuous) that $\mathcal{B}_0 \ni \mathbf{X} \xrightarrow{\tilde{\mathbf{F}}^{ph}} \mathbf{F}^{ph} = \tilde{\mathbf{F}}^{ph}(\mathbf{X}) \in \operatorname{Hom}(T_{\mathbf{x}}\mathcal{B}, T_{\mathbf{x}}\tilde{\mathbf{x}}^{ph}(\mathcal{B}))$. The map $\tilde{\mathbf{x}}'$ describes the shift of the centre of mass of the crystalline cell itself from its current (in a certain sense, "apparent") place \mathbf{x} to another place \mathbf{x}' due to local rearrangements of atoms.

Finally, we indicate by $\dot{\mathbf{x}} = \frac{d}{dt}\tilde{\mathbf{x}}(\mathbf{X}, t)$ and $\dot{\mathbf{w}} = \frac{d}{dt}\tilde{\mathbf{w}}(\mathbf{X}, t)$ rates in the reference description and might also use $\dot{\mathbf{u}} = \frac{d}{dt}\tilde{\mathbf{u}}(\mathbf{X}, t)$ instead of $\dot{\mathbf{x}}$ to put in evidence the role of phonon and phason degrees of freedom.

If we restrict our attention to the infinitesimal deformation regime in which \mathcal{B} can be "confused" with \mathcal{B}_0 in the sense that $\dot{\mathbf{x}} \approx \mathbf{u}$ at each \mathbf{X} , in addition to the standard compatibility condition *curl curl sym* $\nabla \mathbf{u} = \mathbf{0}$, we also get a *phason compatibility condition curl curl* $\nabla \mathbf{w} = \mathbf{0}$ that would eventually imply an energetic contribution of the phason spin.

2.2. Observers and Relabeling

Here we define an observer as a "representation" of all geometrical environments necessary to describe a given body and its motion (see [27]).

The geometrical picture of a quasi-periodic alloy involves the point space \mathcal{E}^3 (i.e., the ambient space), the translation space \mathbb{V}_w (containing phason degrees of freedom), the interval of time $[0, \bar{t}]$, and the fit region \mathcal{B}_0 . An observer \mathcal{O} is then a representation of $\mathcal{E}^3, \mathbb{V}_w, [0, \bar{t}]$, and \mathcal{B}_0 .

The attention is here focused on the ones that I call synchronous semiclassical observers, i.e. observers that "evaluate" with one another the same representation of \mathcal{B}_0 and $[0, \bar{t}]$.

Changes in synchronous semiclassical observers. With the premises above, a generic change in synchronous semiclassical observers involves only a couple of transformations: one of the ambient space \mathcal{E}^3 , the other of \mathbb{V}_w . They are described respectively by the parametrized families of mappings defined below, smooth with respect to the relevant parameter.

- $\mathbb{R}^+ \ni s_2 \longmapsto \mathbf{f}_{s_2}^2 \in Aut(\mathcal{E}^3)$, with \mathbf{f}_0^2 the identity. We put $\mathbf{f}_0^{2'}(\mathbf{X}) = \mathbf{v}$, where the prime denotes differentiation with respect to the parameter.
- A Lie group G, with Lie algebra g, acts over V_w. If ξ ∈ g, its action over w ∈ V_w is denoted by ξ_{V_w} (w). By indicating by w_g the value of w after the action¹ of g ∈ G, if we consider a one-parameter smooth curve ℝ⁺ ∋ s₃ → g_{s₃} ∈ G over G such that ξ = dg_{s₃}/ds₃ |_{s₃=0} and its corresponding orbit s₃ → w<sub>g_{s₃} over V_w, starting from a given w, we have ξ_{V_w} (w) = d/ds₃ w<sub>g_{s₃} |_{s₃=0}.
 </sub></sub>

¹ It is not essential to render precisely whether the action is from the left or from the right.

In other words, two observers connected by the changes defined above differ in the representation of the ambient space by arbitrary (sufficiently smooth) "deformative motions" while in the representation of \mathbb{V}_w by the action of an arbitrary Lie group. Of course one obtains standard changes in observers ruled by rigid body motions when the automorphisms altering the ambient space \mathcal{E}^3 are only isometries, induced by the action of SO(3), and the same copy of SO(3) acts also on \mathbb{V}_w .

Another type of transformation is involved in the developments below: the *relabeling* of the reference place \mathcal{B}_0 . Actually, each observer evaluates the same \mathcal{B}_0 , but one may imagine permuting the possible inhomogeneities in \mathcal{B}_0 itself and require invariance with respect to these "permutations." Formally one may act by relabeling the points of \mathcal{B}_0 by means of the action of the special group of isochoric diffeomorphisms. In other words, one requires invariance (specifically invariance of the Lagrangian density) with respect to the superposition of arbitrary isochoric "deformations" of the reference place. Such a requirement implies invariance with respect to a redistribution of possible defects.

Relabeling. The special group of isochoric point-valued diffeomorphisms *SDiff* acts on \mathcal{B}_0 . Such an action is represented by means of arbitrary smooth curves over *SDiff* (\mathcal{B}_0) emanating from the identity and given formally by

• $\mathbb{R}^+ \ni s_1 \longmapsto \mathbf{f}_{s_1}^1 \in SDiff(\mathcal{B}_0)$, with \mathbf{f}_0^1 the identity.

At each s_1 one finds $\mathbf{X} \mapsto \mathbf{f}_{s_1}^1(\mathbf{X})$, with $Div \mathbf{f}_{s_1}^{1'}(\mathbf{X}) = 0$. We put $\mathbf{f}_0^{1'}(\mathbf{X}) = \mathfrak{v}$.

3. Variational Orinciple for Phonon-Phason Interactions

In constructing a mechanical model of a body, after the description of its morphology, where only geometry is involved, one discusses the representation of interactions and the explicit structure of constitutive laws. The two issues are essentially separated. The representation of interactions by means of appropriate vectors or higher-order tensors is a consequence of the geometrical description of the body: Interactions are in fact entities power-conjugated with the rates of morphological descriptors, and their balance is independent of the constitutive nature of the material.

When we follow a variational approach involving Lagrangian and Hamiltonian formalism, in introducing the Lagrangian density, we put on the same ground the representation of interactions and constitutive laws because they are mixed in the variational description.

Let us consider a fiber bundle,

$$\pi: \mathcal{Y} \to \mathcal{B}_0 \times \left[0, \bar{t}\right],\tag{1}$$

such that $\pi^{-1}(\mathbf{X}, t) = \mathcal{E}^3 \times \mathbb{V}_w$ is the prototype fiber. A generic section $\eta \in \Gamma(\mathcal{Y})$ is then a mapping $\eta : \mathcal{B}_0 \times [0, \bar{t}] \longrightarrow \mathcal{Y}$ such that $\eta(\mathbf{X}, t) = (\mathbf{X}, t, \mathbf{x}, \mathbf{w})$ with \mathbf{x} and \mathbf{w} in the fiber $\pi^{-1}(\mathbf{X}, t)$. If sufficient smoothness for sections is allowed, the first jet bundle $J^1\mathcal{Y}$ over \mathcal{Y} is given by

$$J^{1}\mathcal{Y} \ni j^{1}(\eta) \left(\mathbf{X}, t \right) = \left(\mathbf{X}, t, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{F}, \mathbf{w}, \dot{\mathbf{w}}, \nabla \mathbf{w} \right).$$
(2)

In the conservative case, we presume that the canonical Lagrangian 3 + 1 form

$$L_{\varepsilon}: J^{1}\mathcal{Y} \to \wedge^{3+1} \left(\mathcal{B}_{0} \times \left[0, \bar{t} \right] \right)$$
(3)

admits such a sufficiently smooth density $\mathcal{L}_{\varepsilon}$ that

$$L_{\epsilon}\left(j^{1}\left(\eta\right)\left(\mathbf{X},t\right)\right) = \mathcal{L}_{\varepsilon}d^{3}\mathbf{X}\wedge dt,\tag{4}$$

with $\mathcal{L}_{\varepsilon}$ the value of a map $\tilde{\mathcal{L}}_{\varepsilon}$ (·), namely,

$$\mathcal{L}_{\varepsilon} = \tilde{\mathcal{L}}_{\varepsilon} \left(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{F}, w, \dot{\mathbf{w}}, \nabla \mathbf{w} \right) = \frac{1}{2} \rho_0 \left| \dot{\mathbf{x}} \right|^2 + \frac{1}{2} \varepsilon_1 \bar{\rho} \left| \dot{\mathbf{w}} \right|^2 - \rho_0 \tilde{e}_{\varepsilon_1 \varepsilon_2} \left(\mathbf{X}, \mathbf{F}, \mathbf{w}, \nabla \mathbf{w} \right) - \rho_0 w \left(\mathbf{x} \right),$$
(5)

where ρ_0 is the referential mass density (conserved during the motion), $\bar{\rho}$ the inertia coefficient of possible phason kinetics, *e* the elastic energy density, and *w* the density of the potential of external actions, all per unit mass. Finally, ε_1 and ε_2 are parameters belonging to {0, 1}: Their role is specified below. We write $\mathcal{L}_{\varepsilon}$ instead of $\mathcal{L}_{\varepsilon_1\varepsilon_2}$ for the sake of brevity and will use at times ε in the subscript position with the same meaning. Finally, we do not consider here potential bulk external direct actions on phason changes.

Our attention is focused on the mechanics of quasi-periodic alloys that can be described by a variational principle of the form

$$\delta\left(\int_{\mathcal{B}_0\times[0,\bar{t}]}\mathcal{L}_{\varepsilon}\left(j^1\left(\eta\right)\left(\mathbf{X},t\right)\right)\,d^3\mathbf{X}\wedge dt\right)+(1-\varepsilon_2)\int_{\mathcal{B}_0\times[0,\bar{t}]}\mathbf{z}^{v}\cdot\delta\mathbf{w}\,d^3\mathbf{X}\wedge dt=0,\ (6)$$

where $\mathbf{z}^{v} = \tilde{\mathbf{z}}^{v} (\mathbf{F}, \mathbf{w}, \nabla \mathbf{w}, \dot{\mathbf{w}}) \in T_{\mathbf{w}}^{*} \mathbb{V}_{w}$ accounts for phason friction and is intrinsically dissipative in the sense that

$$\mathbf{z}^{\boldsymbol{v}} \cdot \dot{\mathbf{w}} \ge \mathbf{0},\tag{7}$$

for any choice of $\dot{\mathbf{w}}$. A possible solution of the previous inequality is given by

$$\mathbf{z}^{\nu} = c \dot{\mathbf{w}}^{\flat}, \tag{8}$$

with $\dot{\mathbf{w}}^{\flat}$ the one-form associated with $\dot{\mathbf{w}}$, a form that we identify with $\dot{\mathbf{w}}$ itself for the sake of simplicity, and $c = \tilde{c} (\mathbf{F}, \mathbf{w}, \nabla \mathbf{w}, \dot{\mathbf{w}})$ with \tilde{c} such a scalar definite positive function that

$$\tilde{c}\left(\mathbf{F}, \mathbf{w}, \nabla \mathbf{w}, 0\right) = 0. \tag{9}$$

Actually, a general solution to (7) is given by $\mathbf{z}^v = \mathbf{A}\dot{\mathbf{w}}$, with \mathbf{A} a semidefinite positive second-order tensor (the value of a tensor function of the local state and the phason rate, a function analogous to \tilde{c}), but we restrict our attention to (8) for the sake of simplicity, while keeping in mind the case $\mathbf{A}\dot{\mathbf{w}}$ because the results below also hold for it.

The variational principle (6) is a Lagrange-d'Alambert principle accounting for nonconservative effects (see on this matter [3]). The parametrization of (6) by means of ε_1 and ε_2 allows us to represent the mechanics of quasi-periodic alloys from a unitary standpoint. Namely, since ε_1 and ε_2 take values 0 and 1 only (they are elements of {0, 1}), the cases listed below may occur.

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1. For $\varepsilon_1 = 0$ and $\varepsilon_2 = 0$, (6) reduces formally to

$$\delta\left(\int_{\mathcal{B}_0\times[0,\bar{t}]}\tilde{\mathcal{L}}_0\left(\mathbf{X},\mathbf{x},\mathbf{x},\dot{\mathbf{F}},\mathbf{w},\nabla\mathbf{w}\right)\,d^3\mathbf{X}\wedge dt\right)+\int_{\mathcal{B}_0\times[0,\bar{t}]}\mathbf{z}^{\nu}\cdot\delta\mathbf{w}\,d^3\mathbf{X}\wedge dt=0,\quad(10)$$

where we put

$$e_{00} = \tilde{e}_{00} \left(\mathbf{X}, \mathbf{F}, \nabla \mathbf{w} \right). \tag{11}$$

This kind of variational principle covers the case of quasicrystals where only macroscopic kinetic energy appears. The absence of kinetic energy of a phason nature is suggested by experimental results. In fact, the analysis of diffractions patterns, obtained by exciting a quasi-crystalline specimen by means of X-ray beams, reveals only three soundlike branches associated with standard phonon modes (see [34], [36]). Phason changes are only of diffusive nature, as pointed out by the presence of $\mathbf{z}^v = c\dot{\mathbf{w}}$, which might not depend on \mathbf{w} alone because just $\nabla \mathbf{w}$ is associated with energetic changes in quasicrystals, so that we would get $\mathbf{z}^v = \tilde{\mathbf{z}}^v$ ($\mathbf{F}, \nabla \mathbf{w}, \dot{\mathbf{w}}$).

2. For $\varepsilon_1 = 1$ and $\varepsilon_2 = 1$, (6) reduces to

$$\delta\left(\int_{\mathcal{B}_0\times[0,\bar{t}]}\tilde{\mathcal{L}}_1\left(\mathbf{X},\mathbf{x},\dot{\mathbf{x}},\mathbf{F},\mathbf{w},\dot{\mathbf{w}},\nabla\mathbf{w}\right)\ d^3\mathbf{X}\wedge dt\right)=0,\tag{12}$$

which describes the pure elastic behavior of both IIC and IMC by taking into account phason kinetics. Moreover, for the elastic energy we get

$$e_{11} = \tilde{e}_{11} \left(\mathbf{X}, \mathbf{F}, \mathbf{w}, \nabla \mathbf{w} \right).$$
⁽¹³⁾

Phason friction is not accounted for.

3. For $\varepsilon_1 = 0$ and $\varepsilon_2 = 1$, (6) reduces to

$$\delta\left(\int_{\mathcal{B}_0\times[0,\bar{t}]}\tilde{\mathcal{L}}_{01}\left(\mathbf{X},\mathbf{x},\dot{\mathbf{x}},\mathbf{F},\mathbf{w},\nabla\mathbf{w}\right)\ d^3\mathbf{X}\wedge dt\right)=0,\tag{14}$$

with

$$e_{01} = e_{11}.\tag{15}$$

This variational principle describes the pure elastic behavior of both IIC and IMC when phason kinetics is neglected. Even in this case one does not account for phason friction.

4. For $\varepsilon_1 = 1$ and $\varepsilon_2 = 0$, (6) reduces to

$$\delta\left(\int_{\mathcal{B}_0\times[0,\bar{t}]}\tilde{\mathcal{L}}_{10}\left(\mathbf{X},\mathbf{x},\dot{\mathbf{x}},\mathbf{F},\mathbf{w},\dot{\mathbf{w}},\nabla\mathbf{w}\right) d^3\mathbf{X}\wedge dt\right) + \int_{\mathcal{B}_0\times[0,\bar{t}]} \mathbf{z}^{\nu}\cdot\delta\mathbf{w} d^3\mathbf{X}\wedge dt = 0,$$
(16)

with

$$e_{10} = e_{11}.\tag{17}$$

This variational principle describes the mechanical behavior of both IIC and IMC when both phason inertia and phason friction are considered.

Remark 1. The idea of parametrizing (6) by means of ε_1 and ε_2 , to cover various cases of physical interest, accrues from a similar point of view adopted in geophysical fluid dynamics where, in stratified flows, the kinetic energy in the "vertical" direction is weighed by a parameter ε (see [16]).

The evaluation of the variations in (6) is a standard job, so that one gets appropriate Euler-Lagrange equations under sufficient smoothness of $\mathcal{L}_{\varepsilon}$, namely,

$$\overline{\partial_{\dot{\mathbf{x}}}\mathcal{L}_{\varepsilon}} = \partial_{\mathbf{x}}\mathcal{L}_{\varepsilon} - Div\,\partial_{\mathbf{F}}\mathcal{L}_{\varepsilon},\tag{18}$$

$$\overline{\partial_{\dot{\mathbf{w}}}\mathcal{L}}_{\varepsilon} = \partial_{\mathbf{w}}\mathcal{L}_{\varepsilon} - Div\,\partial_{\nabla\mathbf{w}}\mathcal{L}_{\varepsilon} - (1 - \varepsilon_2)\,\mathbf{z}^{\upsilon}.$$
(19)

Definition 1 (invariance of $\mathcal{L}_{\varepsilon}$). $\mathcal{L}_{\varepsilon}$ is *invariant* with respect to changes in observers and relabeling, i.e. with respect to the action of $\mathbf{f}_{s_1}^1, \mathbf{f}_{s_2}^2$, and *G*, if

$$\mathcal{L}_{\varepsilon} \left(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{F}, \mathbf{w}, \dot{\mathbf{w}}, \nabla \mathbf{w} \right)$$

= $\tilde{\mathcal{L}}_{\varepsilon} \left(\mathbf{f}^{1}, \mathbf{f}^{2}, \left(grad \, \mathbf{f}^{2} \right) \dot{\mathbf{x}}, \left(grad \, \mathbf{f}^{2} \right) \mathbf{F} \left(\nabla \mathbf{f}^{1} \right)^{-1}, \mathbf{w}_{g}, \dot{\mathbf{w}}_{g}, \left(\nabla \mathbf{w}_{g} \right) \left(\nabla \mathbf{f}^{1} \right)^{-1} \right),$ (20)

where we indicate by \mathbf{f}^1 , \mathbf{f}^2 , and \mathbf{w}_g the values $\mathbf{f}_{s_1}^1(\mathbf{X})$, $\mathbf{f}_{s_2}^2(\mathbf{x})$, $\mathbf{w}_{g_{s_3}}(\mathbf{X})$.

Let us define scalar Q_{ε} , m_{ε} (w) and vector $\mathfrak{F}_{\varepsilon}$ densities given respectively by

$$\mathcal{Q}_{\varepsilon} = \partial_{\dot{\mathbf{x}}} \mathcal{L}_{\varepsilon} \cdot (\mathbf{v} - \mathbf{F} \mathfrak{w}) + \partial_{\dot{\mathbf{w}}} \mathcal{L}_{\varepsilon} \cdot \left(\xi_{\mathbb{V}_{w}} \left(\mathbf{w} \right) - \left(\nabla \mathbf{w} \right) \mathfrak{w} \right),$$
(21)

$$\mathbf{m}_{\varepsilon}\left(\mathbf{w}\right) = (1 - \varepsilon_{2}) \, \mathbf{z}^{\upsilon} \cdot \left(\xi_{\mathbb{V}_{w}}\left(\mathbf{w}\right) - \left(\nabla\mathbf{w}\right) \, \mathfrak{w}\right),\tag{22}$$

$$\mathfrak{F}_{\varepsilon} = \mathcal{L}_{\varepsilon} \mathfrak{w} + (\partial_{\mathbf{F}} \mathcal{L}_{\varepsilon})^{T} \left(\mathbf{v} - \mathbf{F} \mathfrak{w} \right) + (\partial_{\nabla \mathbf{w}} \mathcal{L}_{\varepsilon})^{T} \left(\xi_{\mathbb{V}_{w}} \left(\mathbf{w} \right) - \left(\nabla \mathbf{w} \right) \mathfrak{w} \right).$$
(23)

Theorem 1. If the Lagrangian density $\mathcal{L}_{\varepsilon}$ is invariant under $\mathbf{f}_{s_1}^1, \mathbf{f}_{s_2}^2$, and G (as defined in Section 2.2), for the variational principle (6) we get

$$\dot{\mathcal{Q}}_{\varepsilon} + Div\,\mathfrak{F}_{\varepsilon} - \mathsf{m}_{\varepsilon}\,(\mathbf{w}) = 0. \tag{24}$$

It is a Noether-like theorem valid for the variational principle (6). With respect to the statement of Noether theorem in multifield elasticity for complex bodies discussed in [6] (where everything is developed in conservative setting), here we go beyond traditional borders and *account for the dissipative phason friction*. In this way, the new term \mathbf{m}_{ε} (**w**) appears and is the density of the relative power that the dissipative self-force \mathbf{z}^{v} develops with respect to the difference between the "virtual" rate $\xi_{\mathbb{V}_{w}}$ (**w**) induced by *G* on \mathbb{V}_{w} (i.e. by the change in observer) and the push-forward in $T_{\mathbf{w}}\mathbb{V}_{w}$ of the "virtual" velocity of relabeling.

Proof. The request of invariance of $\mathcal{L}_{\varepsilon}$ is equivalent to imposing

$$\left. \frac{d}{ds_1} \mathcal{L}_{\varepsilon} \right|_{s_1 = 0, s_2 = 0, s_3 = 0} = 0, \tag{25}$$

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$$\frac{d}{ds_2}\mathcal{L}_{\varepsilon}\Big|_{s_1=0,s_2=0,s_3=0} = 0,$$
(26)

$$\frac{d}{ds_3} \mathcal{L}_{\varepsilon} \bigg|_{s_1 = 0, s_2 = 0, s_3 = 0} = 0, \tag{27}$$

which lead to

$$\partial_{\mathbf{X}} \mathcal{L}_{\varepsilon} \cdot \mathfrak{w} - \partial_{\mathbf{F}} \mathcal{L}_{\varepsilon} \cdot (\mathbf{F} \nabla \mathfrak{w}) - \partial_{\nabla \mathbf{w}} \mathcal{L}_{\varepsilon} \cdot ((\nabla \mathbf{w}) \nabla \mathfrak{w}) = 0, \tag{28}$$

$$\partial_{\mathbf{x}} \mathcal{L}_{\varepsilon} \cdot \mathbf{v} + \partial_{\dot{\mathbf{x}}} \mathcal{L}_{\varepsilon} \cdot \left((\operatorname{grad} \mathbf{v}) \, \dot{\mathbf{x}} \right) + \partial_{\mathbf{F}} \mathcal{L}_{\varepsilon} \cdot \left((\operatorname{grad} \mathbf{v}) \, \mathbf{F} \right) = 0, \tag{29}$$

$$\partial_{\mathbf{w}} \mathcal{L}_{\varepsilon} \cdot \xi_{\mathbb{V}_{w}} \left(\mathbf{w} \right) + \partial_{\dot{\mathbf{w}}} \mathcal{L}_{\varepsilon} \cdot \xi'_{\mathbb{V}_{w}} \left(\mathbf{w} \right) + \partial_{\nabla \mathbf{w}} \mathcal{L}_{\varepsilon} \cdot \nabla \xi_{\mathbb{V}_{w}} \left(\mathbf{w} \right) = 0.$$
(30)

We then compute the time derivative of Q_{ε} and the divergence of $\mathfrak{F}_{\varepsilon}$. By using (28)–(30), thanks to the validity of (18) and (19), we get

$$\hat{\mathcal{Q}}_{\varepsilon} + Div \,\mathfrak{F}_{\varepsilon} = (1 - \varepsilon_2) \,\mathbf{z}^v \cdot \left(\xi_{\mathbb{V}_w} \left(\mathbf{w}\right) - \left(\nabla \mathbf{w}\right) \,\mathfrak{w}\right). \tag{31}$$

Remark 2. The proof of Noether theorem relies upon two main ingredients: (i) the invariance of the Lagrangian with respect to the action of certain groups and (ii) Euler-Lagrange equations of the variational principle under examination. In the standard conservative case, say the one of nonlinear elasticity of simple bodies, the two points are strictly interconnected because Euler-Lagrange equations are expressed only in terms of the derivatives of the Lagrangian density. In the nonconservative setting treated here, the special structure of the variational principle under examination generates in the Euler-Lagrange equations the term \mathbf{z}^{v} , which is not related to the Lagrangian density: This is the reason for the occurrence of \mathbf{m}_{ε} (**w**).

When $\mathbf{f}_{s_2}^2$ alone acts on $\mathcal{L}_{\varepsilon}$ leaving **v** *arbitrary*, from (24) we get in covariant way, as a standard result, the balance of phonon interaction (standard Cauchy's balance of momentum)

$$\rho_0 \ddot{\mathbf{x}} = \mathbf{b} + Div \,\mathbf{P},\tag{32}$$

where $\mathbf{P} = -\partial_{\mathbf{F}} \mathcal{L}_{\varepsilon}$ is the first Piola-Kirchhoff stress and $\mathbf{b} = \partial_{\mathbf{x}} \mathcal{L}_{\varepsilon}$ the vector of body forces. At each **X** in \mathcal{B}_0 , **P** maps linearly normal to surfaces through **X** into tensions at **x** in \mathcal{B} . There is then a map $\tilde{\mathbf{P}}$ such that $\mathcal{B}_0 \in \mathbf{X} \longmapsto \mathbf{P} = \tilde{\mathbf{P}}(\mathbf{X}) \in Hom(T_{\mathbf{x}}^*\mathcal{B}_0, T_{\mathbf{x}}^*\mathcal{B})$.

Corollary 1. If G acts alone on $\mathcal{L}_{\varepsilon}$, from (24) and the arbitrariness of G, the balance of phason interactions

$$\varepsilon_1 \bar{\rho} \ddot{\mathbf{w}} = -\mathbf{z} - (1 - \varepsilon_2) \, \mathbf{z}^v + Div \, \mathcal{S} \tag{33}$$

follows. $S = -\partial_{\nabla \mathbf{w}} \mathcal{L}_{\varepsilon}$ represents phason stress due to the relative influence of the phason activity between neighboring material elements; $\mathbf{z} = \rho_0 \partial_{\mathbf{w}} e_{\varepsilon_1 \varepsilon_2}$ (self-force) describes conservative self-interactions of a phason nature within each material element, while \mathbf{z}^v describes the relevant phason friction. At each \mathbf{X} , $S \in Hom(T^*_{\mathbf{X}}\mathcal{B}_0, T^*_{\mathbf{w}}\mathbb{V}_w)$ and

 $\mathbf{z}, \mathbf{z}^{v} \in T_{\mathbf{w}}^{*} \mathbb{V}_{w}$. The phason stress S maps linearly normal to surfaces through \mathbf{X} in \mathcal{B}_{0} into tensions of a phason nature, i.e., elements of $T_{\mathbf{w}}^{*} \mathbb{V}_{w} \simeq \mathbb{R}^{3}$. The balance of phason interactions is covariant thanks to the arbitrariness of G.

(a) For $\varepsilon_1 = 0$ and $\varepsilon_2 = 0$, (33) becomes

$$c\dot{\mathbf{w}} = Div\,\mathcal{S},\tag{34}$$

which is the balance of phason interactions for quasicrystals (b) For $\varepsilon_1 = 1$ and $\varepsilon_2 = 1$, (33) reduces to

$$\bar{\rho}\ddot{\mathbf{w}} = Div\,\mathcal{S} - \mathbf{z},\tag{35}$$

which holds for both IIC and IMC in the absence of phason friction. (c) For $\varepsilon_1 = 0$ and $\varepsilon_2 = 1$, the last balance reduces to

$$Div \,\mathcal{S} - \mathbf{z} = \mathbf{0},\tag{36}$$

which is still valid for both IIC and IMC at equilibrium in the pure elastic setting. (d) Finally, the case $\varepsilon_1 = 1$ and $\varepsilon_2 = 0$ corresponds to

$$\bar{\rho}\ddot{\mathbf{w}} + c\dot{\mathbf{w}} = Div\,\mathcal{S} - \mathbf{z},\tag{37}$$

which holds for both IIC and IMC when both phason inertia and friction are accounted for. Of course phason inertia may be negligible at times; in this case one gets

$$c\dot{\mathbf{w}} = Div\,\mathcal{S} - \mathbf{z}.\tag{38}$$

Corollary 2. Let G = SO(3) and, for any element $\dot{\mathbf{q}} \times of$ its Lie algebra, let $\mathbf{f}_{s_2}^2$ be such that $\mathbf{v} = \dot{\mathbf{q}} \times (\mathbf{x} - \mathbf{x}_0)$ with \mathbf{x}_0 a fixed point in space. From (24) one obtains

$$skw\left(\partial_{\mathbf{F}}e\mathbf{F}^{T}+\mathbf{w}\otimes\left(\partial_{\mathbf{w}}e+\mathbf{z}^{v}\right)+\partial_{\nabla\mathbf{w}}e^{T}\left(\nabla\mathbf{w}\right)\right)=0,$$
(39)

where $skw(\cdot)$ extracts the skew-symmetric part of its argument.

In the absence of phason activity, i.e. for common periodic alloys, (39) reduces to

$$skw\left(\partial_{\mathbf{F}}e\mathbf{F}^{T}\right) = 0,\tag{40}$$

which is the standard requirement that the Cauchy stress be symmetric. Corollary 2 points out that the presence of phason interactions renders nonsymmetric Cauchy stress in a way in which the nonsymmetric part is strictly determined by the phason self-force and the phason stress.

Corollary 3. If $\mathbf{f}_{s_1}^{l}$ alone acts on $\mathcal{L}_{\varepsilon}$, with \mathfrak{w} arbitrary, from (24) one gets

$$\frac{1}{\left(\mathbf{F}^{T}\partial_{\dot{\mathbf{x}}}\mathcal{L}_{\varepsilon}+\nabla\boldsymbol{\nu}^{T}\partial_{\dot{\nu}}\mathcal{L}_{\varepsilon}\right)}+Div\left(\mathbb{P}-\frac{1}{2}\left(\rho_{0}\left|\dot{\mathbf{x}}\right|^{2}+\varepsilon_{1}\bar{\rho}\left|\dot{\mathbf{w}}\right|^{2}\right)\mathbf{I}\right)-\partial_{\mathbf{X}}\mathcal{L}_{\varepsilon}$$
$$-\left(1-\varepsilon_{2}\right)\left(\nabla\mathbf{w}\right)^{T}\mathbf{z}^{v}+\mathbf{F}^{T}\mathbf{b}=\mathbf{0},$$
(41)

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where $\mathbb{P} = \rho_0 e_{\varepsilon_1 \varepsilon_2} \mathbf{I} - \mathbf{F}^T \mathbf{P} - \nabla \mathbf{w}^T S \in Aut (\mathbb{R}^3)$, with \mathbf{I} the second-order unit tensor, is a generalized Eshelby tensor accounting for phason activity (a special case of the general one obtained in [24]).

The balance (41) involves measures of interaction like \mathbb{P} that play a role in the evolution of defects (as we shall see later in analyzing the evolution of discontinuity surfaces). However, since (41) follows from the sole requirement of invariance with respect to the "permutation" of possible bulk inhomogeneities, no dissipative additional force driving bulk defects appears because at this stage the defects themselves are considered fixed.

Corollary 4. Let G = SO(3) and, for any element $\dot{q} \times of$ its Lie algebra, $\mathbf{f}_{s_1}^1$ is such that $\mathbf{w} = \dot{q} \times (\mathbf{X} - \mathbf{X}_0)$ with \mathbf{X}_0 a fixed point in \mathcal{B}_0 . If the body is homogeneous, and only the special choices of $\mathbf{f}_{s_2}^2$ and G just defined act on $\mathcal{L}_{\varepsilon}$, \mathbb{P} is symmetric.

Remark 3. Notice that, for fixed **w** and ∇ **w**, a standard result of nonlinear elasticity must hold: namely, $e(\cdot, \mathbf{w}, \nabla \mathbf{w})$ cannot be convex in **F** for reasons of *SO* (3) invariance when large deformations occur. The same property needs to be satisfied by $e(\cdot, \nabla \mathbf{w})$ in the case of quasicrystals. In addition, in the so-called unlocked phase in which phonons may have thermal excitation analogous to phonon one, so that phason Debye-Waller contribution can be recognized, we may find quadratic dependence of $\tilde{e}(\mathbf{F}, \nabla \mathbf{w})$ on ∇ **w** (see [18]). Further restrictions on the constitutive structure of the energy can be obtained by using requirements of material objectivity or covariance (see [29] for the relevant treatment in the case of simple bodies); however, the issue is not developed here.

3.1. Universal Phonon-Phason Changes in Quasicrystals with Vanishing Phason Friction

Phason friction is always present in quasicrystals. However, we may imagine that its effects may be neglected at mechanical equilibrium in some special circumstances in which deformation processes develop almost "instantaneously," in the sense that they are faster than the "activation time" of phason friction. In this case we may recognize a universal character of affine deformations.

When we adopt for quasicrystals the point of view leading to the definition of a global displacement $\mathbf{\bar{u}} \in \mathbb{V}_u \oplus \mathbb{V}_w$ (see [8], [17]), as mentioned in Section 2, we say that the deformation is *affine* when \mathbf{F}' does not depend on \mathbf{X} .

Moreover, if we consider deformations that can be controllable only by applied macroscopic tractions, excluding in this way body forces, we call *universal* all deformations that can occur for bodies in a given class.

Theorem 2. Let the mappings $(\mathbf{F}, \nabla \mathbf{w}) \xrightarrow{\tilde{\mathbf{P}}} \mathbf{P} = \tilde{\mathbf{P}}(\mathbf{F}, \nabla \mathbf{w})$ and $(\mathbf{F}, \nabla \mathbf{w}) \xrightarrow{\tilde{\mathcal{S}}} \mathcal{S} = \tilde{\mathcal{S}}(\mathbf{F}, \nabla \mathbf{w})$ admit bounded partial derivatives with respect to their entries and, at each \mathbf{X} ,

$$\det \begin{pmatrix} \partial_{\mathbf{F}} \mathbf{P} & \partial_{\nabla \mathbf{w}} \mathbf{P} \\ \partial_{\mathbf{F}} \mathcal{S} & \partial_{\nabla \mathbf{w}} \mathcal{S} \end{pmatrix} \neq 0.$$
(42)

All universal static deformations of homogeneous (purely) elastic quasicrystals satisfying the restriction (42) are affine.

Such a theorem is in a certain sense a generalization of a standard result in nonlinear elasticity theory of simple bodies (see [1, p. 506]). Here the difference relies upon the circumstance that phason degrees of freedom are involved and one needs to account for condition (42).

Proof. First recall that in absence of body forces and with negligible phason friction, in conditions of homogeneity, the equilibrium equations for quasicrystals read

$$Div \mathbf{P} = 0, \qquad Div \mathcal{S} = 0.$$
 (43)

We have also

$$Div \mathbf{P} = (\partial_{\mathbf{F}} \mathbf{P}) \nabla \mathbf{F} + (\partial_{\nabla \mathbf{w}} \mathbf{P}) \nabla \nabla \mathbf{w} = 0, \tag{44}$$

$$Div S = (\partial_{\mathbf{F}} S) \nabla \mathbf{F} + (\partial_{\nabla \mathbf{w}} S) \nabla \nabla \mathbf{w} = 0,$$
(45)

i.e.,

$$\mathbb{A}_1 \nabla \mathbf{F} + \mathbb{A}_2 \nabla \nabla \mathbf{w} = 0, \tag{46}$$

$$\mathbb{A}_3 \nabla \mathbf{F} + \mathbb{A}_4 \nabla \nabla \mathbf{w} = 0, \tag{47}$$

with \mathbb{A}_i 's fourth-order tensors that are arbitrary because the explicit form of the mappings $\tilde{\mathbf{P}}$ and $\tilde{\mathcal{S}}$ is not specified. They are also constant because the material is homogeneous. Consequently, thanks to (42), the solution to (46) and (47) provides $\nabla \mathbf{F} = 0$ and $\nabla \nabla \mathbf{w} = 0$, i.e., \mathbf{F} and $\nabla \mathbf{w}$ must be constant. As a consequence, thanks to the additive decomposition, $\mathbf{F}' = \mathbf{F} + \nabla \mathbf{w}$, \mathbf{F}' is constant as well.

3.2. Mutations of Material Metric

The extended Eshelby tensor $\mathbb{P} = \rho_0 e_{\varepsilon_1 \varepsilon_2} \mathbf{I} - \mathbf{F}^T \mathbf{P} - \nabla \mathbf{w}^T S$, accounting for phason effects, appears in the picture of the interactions involved in mutations (such as evolution of defects, interfaces, etc.) [24]. These mutations may be represented by means of "alterations" of the geometrical structure of \mathcal{B}_0 , which, in contrast, would remain fixed once and for all. In particular, we focus our attention here only on mutations that may involve changes in the material metric γ , as it occurs in plastic flows (see [31]) or in the alteration of possible prestressed states (see, e.g., [26]). From now on we assume in this section $\rho_0 = 1$ for notational convenience.

We then consider (with some slight abuse of notation) a density of elastic energy of the form

$$e = \tilde{e} \left(\gamma, \mathbf{F}, \mathbf{w}, \nabla \mathbf{w} \right), \tag{48}$$

in which we express explicitly the presence of γ and require that \tilde{e} be invariant under the action of the group of point-valued diffeomorphisms defined on \mathcal{B}_0 and altering it. The previous choice of the energy is valid for IIC and IMC. Namely, here $e = e_{11} = e_{01} = e_{10}$, as introduced previously in displaying special cases of $e_{\epsilon_1\epsilon_2}$.

In other words, we require that \tilde{e} be invariant under *virtual* superposition of sufficiently smooth deformations altering the reference configuration. Notice that this kind of requirement of invariance is more stringent than the one with respect to relabeling because here it is not required that the diffeomorphisms involved be isochoric.

We then consider a one-parameter family \mathbf{h}_s of sufficiently smooth point-valued diffeomorphisms defined over \mathcal{B}_0 and indicate by \mathbf{u} and \mathbf{H}_s the derivatives $\frac{d}{ds}\mathbf{h}_s|_{s=0}$ and $\nabla \mathbf{h}_s$, respectively. After the action of \mathbf{h}_s , the density *e* changes as

$$e \stackrel{\mathbf{h}_{s}}{\longmapsto} e_{\mathbf{h}_{s}} = (\det \mathbf{H}_{s}) \,\tilde{e} \left(\mathbf{H}_{s}^{-T} \boldsymbol{\gamma} \mathbf{H}_{s}^{-1}, \mathbf{F} \mathbf{H}_{s}^{-1}, \mathbf{w}, (\nabla \mathbf{w}) \, \mathbf{H}_{s}^{-1} \right).$$
(49)

Theorem 3. If the energy density e depends on the metric γ in \mathcal{B}_0 and is invariant in the sense defined above, we get

$$\mathbb{P}_{B}^{A} = 2 \left(\partial_{\gamma} e \right)^{AC} \gamma_{CB}.$$
(50)

Proof. The proof relies upon the circumstance that the requirement of invariance of *e* under the action of \mathbf{h}_s implies $\frac{d}{ds}e_{\mathbf{h}_s}|_{s=0}$, i.e.,

$$\tilde{e}(\gamma, \mathbf{F}, \mathbf{w}, \nabla \mathbf{w}) tr \nabla \mathfrak{u} - \partial_{\gamma} e \cdot \left((\nabla \mathfrak{u})^{T} \gamma + \gamma (\nabla \mathfrak{u}) \right) - \partial_{\mathbf{F}} e \cdot \mathbf{F} \nabla \mathfrak{u} - \partial_{\nabla \mathbf{w}} e \cdot (\nabla \mathbf{w}) \nabla \mathfrak{u} = 0,$$
(51)

since $\frac{d}{ds}\mathbf{H}_s^{-1}|_{s=0} = -\nabla \mathfrak{u}$. As a consequence of the symmetry of γ , we then get

$$\left(e\mathbf{I} - \mathbf{F}^{T}\mathbf{P} - \nabla \mathbf{w}^{T}\mathcal{S} - 2\left(\partial_{\gamma} e\right)\boldsymbol{\gamma}\right) \cdot \nabla \boldsymbol{\mathfrak{u}} = 0,$$
(52)

which implies (50), thanks to the arbitrariness of ∇u .

The result in Theorem 3 is the counterpart for the extended Eshelby stress \mathbb{P} of Doyle-Ericksen formula valid for Cauchy stress in the mechanics of simple bodies. The Doyle-Ericksen formula tells us that Cauchy stress is generated by the variations of the energy with respect to the variations of the spatial metric (remember for further clarification that the right Cauchy-Green tensor **C** is the pull-back in \mathcal{B}_0 of the spatial metric **g** by means of the deformation $\tilde{\mathbf{x}}$). In the same way, Theorem 3 states that the tensor \mathbb{P} is associated with the variation of the energy with respect to the variations of the material metric, variations determined by changes in the defect structure. In this sense, Theorem 3 enforces the physical meaning attributed to the balance (41).

Remark 4. Notice that

$$\mathbb{P}^{AD} = \mathbb{P}^{A}_{B} \gamma^{BD} = 2 \left(\partial_{\gamma} e \right)^{AC} \gamma_{CB} \gamma^{BD} = 2 \left(\partial_{\gamma} e \right)^{AD}$$
(53)

is symmetric since γ does.

Remark 5. Notice also that the result of Theorem 3 is also valid for quasicrystals. In fact, in the proof above, **w** plays just a parametric role.

4. Elementary Hamiltonian Structures for IIC and IMC

For IIC and IMC, Hamiltonian structures follow in a natural way. Here we restrict our treatment to the case in which phason inertia is accounted for and write \mathcal{L} instead of \mathcal{L}_1 for notational convenience.

Let **p** and μ be respectively the *canonical momentum* and the *canonical phason* momentum defined respectively by $\mathbf{p} = \partial_{\dot{\mathbf{x}}} \mathcal{L}$ and $\mu = \partial_{\dot{\mathbf{w}}} \mathcal{L}$. The Hamiltonian density \mathcal{H} is then given by

$$\mathcal{H}(\mathbf{X}, \mathbf{x}, \mathbf{p}, \mathbf{F}, \mathbf{w}, \boldsymbol{\mu}, \nabla \mathbf{w}) = \mathbf{p} \cdot \dot{\mathbf{x}} + \boldsymbol{\mu} \cdot \dot{\mathbf{w}} - \mathcal{L}(\mathbf{X}, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{F}, \mathbf{w}, \dot{\mathbf{w}}, \nabla \mathbf{w}).$$
(54)

In terms of partial derivatives of \mathcal{H} , the balances (18) and (19) with $\varepsilon_1 = 1$ and $\varepsilon_2 = 1$ can be written as

$$\dot{\mathbf{p}} = -\partial_{\mathbf{x}}\mathcal{H} + Div\,\partial_{\mathbf{F}}\mathcal{H},$$

$$\dot{\mathbf{x}} = \partial_{\mathbf{p}}\mathcal{H},$$
(55)

$$\dot{\boldsymbol{\mu}} = -\partial_{\mathbf{w}} \mathcal{H} + Div \,\partial_{\nabla \mathbf{w}} \mathcal{H},$$

$$\dot{\mathbf{w}} = \partial_{\boldsymbol{\mu}} \mathcal{H},$$
(56)

which are Hamilton equations for both IIC and IMC when phason inertia occur and phason friction is neglected. General boundary conditions of the type

$$\mathbf{x}\left(\mathbf{X}\right) = \bar{\mathbf{x}} \quad \text{on } \partial^{(\mathbf{x})} \mathcal{B}_0, \tag{57}$$

$$\partial_{\mathbf{F}} \mathcal{H} \mathbf{n} = \mathbf{t} \quad \text{on } \partial^{(\mathbf{t})} \mathcal{B}_0,$$
 (58)

$$\mathbf{w}\left(\mathbf{X}\right) = \bar{\mathbf{w}} \quad \text{on } \partial^{(\mathbf{w})} \mathcal{B}_{0}, \tag{59}$$

$$\partial_{\nabla \mathbf{w}} \mathcal{H} \mathbf{n} = \mathbf{t} \quad \text{on } \partial^{(\mathfrak{t})} \mathcal{B}_0$$
 (60)

hold, where $\bar{\mathbf{x}}$, \mathbf{t} , $\bar{\mathbf{w}}$, and \mathbf{t} are prescribed on the relevant parts $\partial^{(\cdot)}\mathcal{B}_0$ of the boundary, chosen to be such that $\partial^{(\mathbf{x})}\mathcal{B}_0 \cap \partial^{(\mathbf{t})}\mathcal{B}_0 = \emptyset$ with $Cl(\partial \mathcal{B}_0) = Cl(\partial^{(\mathbf{x})}\mathcal{B}_0 \cup \partial^{(\mathbf{t})}\mathcal{B}_0)$, and $\partial^{(\mathbf{w})}\mathcal{B}_0 \cap \partial^{(\mathbf{t})}\mathcal{B}_0 = \emptyset$ with $Cl(\partial \mathcal{B}_0) = Cl(\partial^{(\mathbf{v})}\mathcal{B}_0 \cup \partial^{(\mathbf{t})}\mathcal{B}_0)$, where Cl indicates closure and \mathbf{n} is the outward unit normal to $\partial \mathcal{B}_0$ at all points in which it is well defined.

Hamilton equations above are special cases of the ones discussed in [6], where morphological descriptors selected as elements of an abstract manifold are accounted for to describe general complex bodies.

It is rather difficult to imagine a loading device prescribing phason tractions t at the boundary. Problems with traction data might thus involve the existence of at least one surface density $U(\mathbf{w})$ such that $\mathbf{t} = \rho_0 \partial_{\mathbf{w}} U$ and another density of the type $\overline{U}(\mathbf{x})$ with $\mathbf{t} = \rho_0 \partial_{\mathbf{x}} \overline{U}$. In this way one considers the external boundary as a structured surface enveloping the body.

In this case, the Hamiltonian H of the whole body is then given by

$$H(\mathbf{x}, \mathbf{p}, \mathbf{w}, \boldsymbol{\mu}) = \int_{\mathcal{B}_0} \mathcal{H}(\mathbf{X}, \mathbf{x}, \mathbf{p}, \mathbf{w}, \boldsymbol{\mu}) d^3 \mathbf{X}$$
$$-\int_{\partial^{(2)} \mathcal{B}_0} \left(\bar{\mathbf{U}}(\mathbf{x}) - \mathbf{U}(\mathbf{w}) \right) d\mathfrak{H}^2, \tag{61}$$

where $\partial^{(2)}\mathcal{B}_0 = \partial^{(t)}\mathcal{B}_0 \cup \partial^{(t)}\mathcal{B}_0$ and $d\mathfrak{H}^2$ is the two-dimensional Hausdorff measure over $\partial^{(2)}\mathcal{B}_0$. Notice that we write $\mathcal{H}(\mathbf{X}, \mathbf{x}, \mathbf{p}, \mathbf{w}, \mu)$ instead of $\mathcal{H}(\mathbf{X}, \mathbf{x}, \mathbf{p}, \mathbf{F}, \mathbf{w}, \mu, \nabla \mathbf{w})$ because below we consider directly variational derivatives.

Theorem 4. The canonical Hamilton equation

$$\dot{F} = \{F, H\} \tag{62}$$

is equivalent to the Hamiltonian system of balance equations (55)–(56) for both IIC and IMC, where F is any functional of the type $\int_{\mathcal{B}_0} f(\mathbf{X}, \mathbf{x}, \mathbf{p}, \mathbf{w}, \boldsymbol{\mu})$, with f a sufficiently smooth scalar density, and the bracket $\{\cdot, \cdot\}$ is defined by

$$\{F, H\} = \int_{\mathcal{B}_{0}} \left(\frac{\delta f}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{p}} - \frac{\delta \mathcal{H}}{\delta \mathbf{x}} \cdot \frac{\delta f}{\delta \mathbf{p}} \right) d^{3}\mathbf{X} + \int_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} \left(\frac{\delta f}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{p}} \Big|_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} - \frac{\delta \mathcal{H}}{\delta \mathbf{x}} \cdot \frac{\delta f}{\delta \mathbf{p}} \Big|_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} \right) d\mathfrak{H}^{2} + \int_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} \left(\frac{\delta f}{\delta \mathbf{w}} \cdot \frac{\delta \mathcal{H}}{\delta \mu} \Big|_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} - \frac{\delta \mathcal{H}}{\delta \mathbf{w}} \cdot \frac{\delta f}{\delta \mu} \Big|_{\partial^{(\mathbf{t})}\mathcal{B}_{0}} \right) d\mathfrak{H}^{2} + \int_{\mathcal{B}_{0}} \left(\frac{\delta f}{\delta \mathbf{w}} \cdot \frac{\delta \mathcal{H}}{\delta \mu} - \frac{\delta \mathcal{H}}{\delta \mathbf{w}} \cdot \frac{\delta f}{\delta \mu} \right) d^{3}\mathbf{X},$$
(63)

where the variational derivative $\frac{\delta \mathcal{H}}{\delta \mathbf{x}}$ is obtained, fixing **p** and allowing **x** to vary; an analogous meaning is valid for the variational derivative with respect to the phason degree of freedom.

The proof follows by direct calculation (a version of this theorem is in [6]).

Remark 6. The bracket $\{\cdot, \cdot\}$ is bilinear and skew-symmetric and satisfies the Jacobi identity.

Remark 7. For F = H, (62) coincides with the equation of conservation of energy.

Let us consider a boundary value problem in which traction data are not prescribed at the boundary, where only conditions like (57) and (59) hold. In this case, (63) reduces to

$$\{F, H\} = \int_{\mathcal{B}_0} \{f, \mathcal{H}\}_P \ d^3 \mathbf{X},\tag{64}$$

where

$$\{f, \mathcal{H}\}_{P} = \left(\frac{\delta f}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{p}} - \frac{\delta \mathcal{H}}{\delta \mathbf{x}} \cdot \frac{\delta f}{\delta \mathbf{p}}\right) + \left(\frac{\delta f}{\delta \mathbf{w}} \cdot \frac{\delta \mathcal{H}}{\delta \mu} - \frac{\delta \mathcal{H}}{\delta \mathbf{w}} \cdot \frac{\delta f}{\delta \mu}\right).$$
(65)

It is simple to verify that $\{\cdot, \cdot\}_P$ is bilinear and skew-symmetric, and satisfies both Jacobi identity and Leibniz identity. Then, $\{\cdot, \cdot\}_P$ induces relevant Poisson structures.

4.1. Purely Spatial Representation

A purely spatial representation of all structures described above is available with all fields defined over \mathcal{B} rather than \mathcal{B}_0 . Then \mathcal{B}_0 does not appear more neither as a reference place nor as a paragon for quantities involved.² In a purely spatial representation we start by assuming for the Hamiltonian density a structure of the form

$$\tilde{\mathcal{H}}(\mathbf{x}, \mathbf{p}, \mathbf{g}, \mathbf{w}_a, \boldsymbol{\mu}_a, \operatorname{grad} \mathbf{w}_a),$$
(66)

where now μ_a is the canonical momentum conjugated with $\dot{\mathbf{w}}_a$ and \mathcal{H} depends also on the spatial metric **g** rather than on the gradient of deformation **F** because no reference to \mathcal{B}_0 is made. In this case, Hamilton equations for both IIC and IMC in pinning free states are given by

$$\dot{\mathbf{p}} = -\partial_{\dot{\mathbf{x}}} \mathcal{H} + div \left(2\partial_{\mathbf{g}} \mathcal{H} - (grad \, \mathbf{w})^T \, \partial_{grad \, \mathbf{w}} \mathcal{H} \right), \dot{\mathbf{x}} = \partial_{\mathbf{p}} \mathcal{H},$$
(67)

$$\dot{\boldsymbol{\mu}} = -\partial_{\dot{\mathbf{w}}} \mathcal{H} + div \,\partial_{grad\,\mathbf{w}} \mathcal{H},$$

$$\dot{\mathbf{w}} = \partial_{\mu} \mathcal{H}.$$
(68)

Here, the Cauchy stress σ is given by

$$\boldsymbol{\sigma} = 2\partial_{\mathbf{g}}\mathcal{H} - (\operatorname{grad} \mathbf{w})^T \,\partial_{\operatorname{grad} \mathbf{w}}\mathcal{H}. \tag{69}$$

Equation (69) is a generalized version of the Doyle-Ericksen formula: The basic difference is the second addendum on the right-hand side, besides the presence of **w** and its gradient in the list of constitutive variables. The term $(grad \mathbf{w})^T \partial_{grad \mathbf{w}} \mathcal{H}$ rules the exchange of energy between the gross scale of macroscopic deformation and the finer scale of phason changes and vice versa. An analogous phenomenon occurs in complex fluids where topological transitions along flows may be generated by this type of energy transfer [25].

5. Dissipative Brackets in the Presence of Phason Friction

The bracket formalism can be extended also to cover dissipative processes such as phason friction. The possible construction of dissipative brackets for various types of nonconservative processes has been discussed variously. We refer mainly to [3], [13], [14], and [15] (see also [2] for dissipation in complex bodies).

To account for phason friction described by \mathbf{z}^{v} , we introduce first a dissipation function \mathcal{R} of the type

$$\mathcal{R} = (1 - \varepsilon_2) \, \frac{1}{2} c \dot{\mathbf{w}}^{\flat} \cdot \boldsymbol{\mu}^{\#}, \tag{70}$$

² For a pure spatial formulation of variational principles, see also [4], [15].

with $\mu^{\#}$ the vector associated with the co-vector μ , a form that we identify with μ itself for the sake of simplicity and write just as $\dot{\mathbf{w}} \cdot \mu$. The global counterpart *R* of \mathcal{R} is given by

$$R = \int_{\mathcal{B}_0} \mathcal{R} d^3 \mathbf{X}.$$
 (71)

Then, we define the bracket $[\cdot, \cdot]$ by

$$[F, R] = -\int_{\mathcal{B}_0} [f, \mathcal{R}]_P d^3 \mathbf{X},$$
(72)

with

$$[f,\mathcal{R}]_P = \frac{\delta f}{\delta \mu} \cdot \frac{\delta \mathcal{R}}{\delta \mu}.$$
(73)

(i) $[\cdot, \cdot]_P$ is symmetric by definition,

(ii) $[\mathcal{R}, \mathcal{R}]_P \geq 0.$

Property (ii) underlines the circumstances that, by definition, $\mathbf{z}^{\nu} = \partial_{\mu} \mathcal{R}$ is intrinsically dissipative.

With these premises, the equations of motion for both IIC and IMC can be put in the form

$$\dot{F} = \{F, H\} + [F, R].$$
 (74)

Remark 8. Since the manifold of substructural shapes is \mathbb{V}_w for quasi-periodic alloys, it could be rather natural to develop appropriate Euler-Poincaré and Lie-Poisson equations, with and without dissipation, by using reduction theory (see [3], [7], [30]) in the form discussed in [15].

6. Linearized Setting

The microstress S, the self-force $\mathbf{z} + \mathbf{z}^v$, and Piola-Kirchhoff stress \mathbf{P} have counterparts defined over \mathcal{B} , namely S_a , $\mathbf{z}_a + \mathbf{z}_a^v$ and Cauchy stress $\boldsymbol{\sigma}$. They are linked with one another by Piola transform, so that one gets

$$\boldsymbol{\sigma} = (\det \mathbf{F})^{-1} \mathbf{P} \mathbf{F}^T, \tag{75}$$

$$\mathcal{S}_a = (\det \mathbf{F})^{-1} \mathcal{S} \mathbf{F}^T, \tag{76}$$

$$\mathbf{z}_a + \mathbf{z}_a^{\nu} = (\det \mathbf{F})^{-1} \left(\mathbf{z} + \mathbf{z}^{\nu} \right).$$
(77)

In the case of infinitesimal deformations and displacements, one may "confuse" \mathcal{B}_0 with \mathcal{B} in the sense that $\left|\frac{\partial x^i}{\partial X^J}\right| \ll 1$ so that

$$\mathbf{P} \approx \boldsymbol{\sigma}, \qquad \mathcal{S} \approx \mathcal{S}_a, \qquad \mathbf{z} + \mathbf{z}^v \approx \mathbf{z}_a + \mathbf{z}_a^v. \tag{78}$$

6.1. Linear Constitutive Equations for Quasicrystals and Their Application to Al_{70.3}Pb_{21.5}Mn_{8.2}

In the case of quasicrystals, the conservative part of the self-force vanishes, i.e. $\mathbf{z} = 0$ (see (34)), while $\mathbf{z}^v = c\dot{\mathbf{w}}$ where *c* can be considered constant. The elastic energy is a quadratic form in $\nabla \mathbf{u}$ and $\nabla \mathbf{w}$, and one gets

$$\boldsymbol{\sigma} = \mathbb{C}\nabla \mathbf{u} + \mathbb{K}' \nabla \mathbf{w},\tag{79}$$

$$\mathcal{S}_a = \mathbb{K}' \nabla \mathbf{u} + \mathbb{K} \nabla \mathbf{w}, \tag{80}$$

where \mathbb{C} , \mathbb{K}' , and \mathbb{K} are constitutive fourth-order tensors. In the case of fivefold symmetry, the constitutive tensors have componentwise expressions given by [17],

$$(\mathbb{C})_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right), \tag{81}$$

$$(\mathbb{K})_{ijkl} = K_1 \delta_{ik} \delta_{jl} + K_2 \left(\delta_{ij} \delta_{kl} - \delta_{il} \delta_{jk} \right), \tag{82}$$

$$\left(\mathbb{K}'\right)_{iikl} = K_3 \left(\delta_{i1} - \delta_{i2}\right) \left(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right),\tag{83}$$

where δ_{ij} is Kronecker symbol and no summation is assumed over repeated indices in the last expression. Substitution of the constitutive laws above in the balance equations, written in terms of actual measures of interactions (σ , S_a , and \mathbf{z}_a^v), allows one to recognize linear theories proposed in the current literature about quasicrystals (see the review article [17]). Basic differences are not in the structure of pointwise balance equations but in their integral counterparts: In Section 8 below we show how integral balances follow naturally from the requirement of *SO* (3) invariance of the power of all (phonon and phason) external actions over any arbitrary part of \mathcal{B}_0 ; they are different from those postulated in [17] even if they furnish the same set of pointwise balances.

Even in the linearized setting one finds results rather surprising. For example, if the constitutive equations above are applied to analyze the behavior of $Al_{70.3}Pb_{21.5}Mn_{8.2}$, exact values of K_1 and K_2 can be found, but there are experimental uncertainties about the value of the coupling coefficient K_3 . For this reason, in analyzing the dynamic problem of propagation of linear waves, one investigates the spectral properties of the associated acoustic tensor (generalized to account for phason effects) by varying K_3 between experimental limits. Relevant numerical analyses have been developed in [28]. Some results are summarized below.

Proposition 1 ([28]). In quasicrystals, the cooperation between phonon and phason modes may generate wave localization (in the sense of standing waves) already in a linear constitutive setting; such a localization may accrue even in the theoretical limit of vanishing phason friction and consequent pure elastic behavior.

Proposition 2 ([28]). In two-dimensional ambient space, in addition to quasilongitudinal and quasi-transversal waves, polarized elliptically, another wave (that we call quasi-phasonic) may arise and is almost spherically polarized: It is a peculiar effect of phonon-phason interaction.

Above, the prefix "quasi-" is used to remind readers that the resulting longitudinal and transversal waves are different from the analogous waves in linear elasticity, due to the influence of phason activity. In the limit case of vanishing phason friction, harmonic waves can propagate only below a critical threshold and the wave localization quoted in Proposition 1 appears. The presence of nonvanishing phason friction eliminates the above-mentioned thresholds. The influence of phason friction is prominent only in a certain range. Moreover, beyond a certain value of phason friction, phason degrees of freedom are essentially frozen. No quasi-phasonic wave exists when phason and phonon wave-vectors are aligned; moreover, it is possible to find localization effects of quasiphasonic waves in the sense of standing waves. Quasi-phasonic and quasi-longitudinal waves interact at certain values of phason friction. Relevant proofs can be found in [28]. These types of results cannot by obtained by making use of the sole setting of the standard linear elasticity of simple bodies.

Of course, the linear theory cannot describe all phenomena that may occur in quasiperiodic alloys. Finite deformations drastically alter the energetic content of each crystalline cell, favouring or obstructing phason activity in a manner different from the one of the infinitesimal deformation regime. The interaction between phonon and phason modes becomes more complex, and a fully nonlinear theory is necessary (see remarks in [33]).

7. Evolution of Wall Defects

Surfaces across which some quantities undergo bounded jumps may occur in quasiperiodic alloys. They may be shock or acceleration waves, dislocations, cracks, and so on (see [23]). To describe their evolution, one needs to account not only for their geometry and the action of standard interactions due to deformation processes, but also for the effects of phason interactions.

Below we consider discontinuity surfaces endowed with their own surface energy. In this way we model the physical circumstance that wall defects are often regions in a metastable state with a high concentration of energy [23]. We allow not only for discontinuities of the standard gradient of deformation **F** across some surface but also for bounded jumps of **w** and its gradient. Really, one may argue that the presence of $\nabla \mathbf{w}$ in the list of entries of the energy takes into account in a regularized way possible grain boundaries and, in general, possible diffused interfaces generated by phason activity. This is true when the grain boundary is between two regions with constant phason activity. However, in the presence of defects or in the presence of subgrains containing "worms" (i.e. the topological alterations of lattices assuring quasiperiodicity in quasicrystals), we may have *interaction between diffuse interfaces and sharp discontinuity surfaces*. This is exactly the situation that we are analyzing here.

7.1. Geometry of a Discontinuity Surface in \mathcal{B}_0

Let Σ be a single surface coinciding with { $\mathbf{X} \in cl\mathcal{B}_0$, $g(\mathbf{X}) = 0$ }, where g is a smooth function (smoothness chosen for the sake of simplicity) with nonsingular gradient. It is oriented by the normal vector field $\mathbf{m} = \tilde{\mathbf{m}}(\mathbf{X}) = \nabla g(\mathbf{X}) / |\nabla g(\mathbf{X})|$.

Let $\mathcal{B}_0 \ni \mathbf{X} \longmapsto a = \tilde{a}(\mathbf{X})$ be a field taking values in a linear space and suffering bounded discontinuities across Σ . For $\eta > 0$ we indicate by a^{\pm} the limits $\lim_{\substack{\eta \to 0 \\ \mathbf{X} \in \Sigma}} a(\mathbf{X} \pm \eta \mathbf{m})$. The jump [a] across Σ is defined by $[a] = a^+ - a^-$, while the

average $\langle a \rangle$ is defined by $2 \langle a \rangle = a^+ + a^-$. If fields a_1 and a_2 have the same properties of a, we have $[a_1a_2] = [a_1] \langle a_2 \rangle + \langle a_1 \rangle [a_2]$ with the product a_1a_2 defined in some way assuring distributivity.

 Σ is *coherent* when at each **X** one gets [**F**] (**I** - **m** \otimes **m**) = **0**.

For any (even "virtual") motion of Σ prescribed by means of a vector field

$$\Sigma \ni \mathbf{X} \stackrel{\varpi}{\longmapsto} \boldsymbol{\varpi} = \tilde{\boldsymbol{\varpi}} \left(\mathbf{X} \right) \in \mathbb{R}^3, \tag{84}$$

with normal component $U = \boldsymbol{\varpi} \cdot \mathbf{m}$, if we assume that the standard velocity $\dot{\mathbf{x}}$ may suffer bounded jumps across $\boldsymbol{\Sigma}$, we get the condition $[\dot{\mathbf{x}}] = -U[\mathbf{F}]\mathbf{m}$.

At each $\mathbf{X} \in \Sigma$ we define the surface deformation gradient \mathbb{F} to be the "projection" over Σ of the average $\langle \mathbf{F} \rangle$, namely,

$$\mathbb{F} = \langle \mathbf{F} \rangle \left(\mathbf{I} - \mathbf{m} \otimes \mathbf{m} \right) \in Hom \left(T_{\mathbf{X}} \Sigma, T_{\mathbf{x}} \mathcal{B} \right), \tag{85}$$

and indicate by \mathbb{N} the projection over Σ of the average of $\nabla \mathbf{w}$, namely,

$$\mathbb{N} = \langle \nabla \mathbf{w} \rangle \left(\mathbf{I} - \mathbf{m} \otimes \mathbf{m} \right) \in Hom \left(T_{\mathbf{X}} \Sigma, T_{\mathbf{w}} \mathbb{V}_{w} \right).$$
(86)

7.2. Phonon and Phason Surface Measures of Interaction and Their Balance

We consider Σ to be endowed with a *surface energy density* ϕ assumed to be sufficiently smooth and given by

$$(\mathbf{m}, \mathbb{F}, \langle \mathbf{w} \rangle, \mathbb{N}) \stackrel{\phi}{\longmapsto} \phi = \tilde{\phi} (\mathbf{m}, \mathbb{F}, \langle \mathbf{w} \rangle, \mathbb{N}).$$
(87)

The dependence of ϕ on **m** accounts for the *anisotropy* of Σ . We require the invariance of ϕ with respect to

(i) changes in observers and

(ii) relabeling of Σ .

As discussed above, changes in observers are characterized by the action of the group of automorphisms of \mathcal{E}^3 and a generic Lie group over \mathbb{V}_w . However, the definition of relabeling needs to be modified because we need $\mathbf{f}_{s_1}^1$ to leave points of Σ over Σ itself and permute them only over the surface.

We should then consider time-parametrized families $s_1 \mapsto \hat{\mathbf{f}}_{s_1}^l$ of elements of *SDiff* (\mathcal{B}_0) characterized by the properties listed below (see [10]).

- 1. The map $s_1 \mapsto \hat{\mathbf{f}}_{s_1}^l$ satisfies the definition of relabeling in Section 2. Moreover, the field $\mathcal{B}_0 \ni \mathbf{X} \mapsto \mathfrak{w} = \tilde{\mathfrak{w}}(\mathbf{X}) = \hat{\mathbf{f}}_0^{l'}(\mathbf{X})$ is at least of class $C^1(\mathcal{B}_0)$. It is then continuous and differentiable across and along Σ .
- 2. Each $\mathbf{f}_{s_1}^{l}$ preserves the elements of area of Σ . Namely, if dA is the element of area of Σ in \mathcal{B}_0 , $dA = \hat{\mathbf{f}}_{s_1}^{l*} \circ dA$, where the asterisk indicates push forward.

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3. $(\nabla \mathfrak{w}) \mathbf{m} = \mathbf{0}$.

4. $\nabla_{\Sigma} \mathbf{v}_m = 0$, with $\mathbf{v}_m = \mathbf{w} \cdot \mathbf{m}$.

Definition 2 (invariance of ϕ). A surface energy density ϕ is invariant with respect to changes in observers and relabeling, i.e. with respect to the action of $\hat{\mathbf{f}}_{s_1}^1, \mathbf{f}_{s_2}^2$ and *G*, if

$$\tilde{\phi}(\mathbf{m}, \mathbb{F}, \langle \mathbf{w} \rangle, \mathbb{N}) = \tilde{\phi}\left(\nabla \hat{\mathbf{f}}^{1T} \mathbf{m}, \left(grad_{\Sigma} \mathbf{f}^{2}\right) \mathbb{F}\left(\nabla \hat{\mathbf{f}}^{1}\right)^{-1}, \langle \mathbf{w} \rangle_{g}, \mathbb{N}_{g}\left(\nabla \hat{\mathbf{f}}^{1}\right)^{-1}\right), \quad (88)$$

for any $g \in G$ and $s_1, s_2 \in \mathbb{R}^+$, where $\mathbb{N}_g = \langle \nabla \mathbf{w}_g \rangle (\mathbf{I} - \mathbf{m} \otimes \mathbf{m})$ and we have used notations common to Definition 1.

Let \mathfrak{X} be a sufficiently smooth vector density defined over Σ by

$$\mathfrak{X} = -\phi \Pi \mathbf{w} + (\partial_{\mathbb{F}} \phi)^T \left(\mathbf{v} - \langle \mathbf{F} \rangle \mathfrak{w} \right) + (\partial_{\mathbb{N}} \phi)^T \left(\xi_{\mathbb{V}_{\mathbf{w}}} \left(\langle \mathbf{w} \rangle \right) - \langle \nabla \mathbf{w} \rangle \mathfrak{w} \right) - (\partial_{\mathbf{m}} \phi \otimes \mathbf{m}) \mathfrak{w}.$$
(89)

This is the surface counterpart of \mathfrak{F} . No surface counterpart of \mathcal{Q} exists, because Σ has no intrinsic inertia relative to the rest of the body (see [10] for additional details about the nature of \mathfrak{X} for general complex bodies).

We consider surface effects of phason friction given by a *surface self-force* \mathfrak{z}^{ν} which is over Σ the counterpart of \mathbf{z}^{ν} . It is intrinsically dissipative in the sense that

$$\mathbf{\mathfrak{z}}^{\boldsymbol{v}}\cdot\mathbf{w}^{\leq}\geq0,\tag{90}$$

for any choice of the rate $\mathbf{w}^{\triangleleft}$, i.e. the rate of **w** following the motion of Σ , and given by

$$\mathbf{w}^{\leq} = \langle \dot{\mathbf{w}} \rangle + \langle \nabla \mathbf{w} \rangle \,\boldsymbol{\varpi}. \tag{91}$$

We presume that \mathfrak{z}^{ν} has a constitutive structure of the type

$$\mathfrak{z}^{\nu} = \tilde{\mathfrak{z}}^{\nu} \left(\mathbf{m}, \mathbb{F}, \langle \mathbf{w} \rangle, \mathbb{N}, \mathbf{w}^{\leq} \right) \in T^*_{\langle \mathbf{w} \rangle} \mathbb{V}_w, \tag{92}$$

so that a solution of the inequality (90) is

$$\mathfrak{z}^{\nu} = \mathfrak{a} \mathbf{w}^{\leq \flat},\tag{93}$$

with $\mathbf{w}^{\leq b}$ the one form associated with \mathbf{w}^{\leq} (a form that we identify with \mathbf{w}^{\leq} for the sake of simplicity) and \mathfrak{a} the value $\mathfrak{a} = \check{\mathfrak{a}} (\mathbf{m}, \mathbb{F}, \langle \mathbf{w} \rangle, \mathbb{N}, \mathbf{w}^{\leq})$ of a definite positive scalar function $\check{\mathfrak{a}}$ (·).

We then define n_{ε} ($\langle \mathbf{w} \rangle$) by

$$n_{\varepsilon}\left(\langle \mathbf{w} \rangle\right) = (1 - \varepsilon_2) \,\mathfrak{z}^{\upsilon} \cdot \left(\xi_{\mathbb{V}_{\mathbf{w}}}\left(\langle \mathbf{w} \rangle\right) - \langle \nabla \mathbf{w} \rangle \,\mathfrak{w}\right). \tag{94}$$

It is the "relative" power developed by \mathfrak{z}^v in the difference between the rate induced by G on \mathbb{V}_w at $\langle \mathbf{w} \rangle$ and the push-forward on \mathbb{V}_w of the virtual velocity of relabeling.

When the motion of Σ , described by the vector field $\tilde{\varpi}$, is not virtual—rather it is the *real* irreversible motion of Σ with respect to \mathcal{B}_0 —dissipation is associated with such an evolution, during which we presume that Σ remains coherent. A dissipative *surface*

driving force \mathbf{f}_{Σ} along Σ occurs; coherence allows us to write the condition of dissipation for \mathbf{f}_{Σ} only on the normal component to Σ , so that we require

$$(\mathbf{f}_{\Sigma} \cdot \mathbf{m}) \ U \le 0, \tag{95}$$

for any choice of U. Such a condition implies that the normal component $f_{\Sigma} = \mathbf{f}_{\Sigma} \cdot \mathbf{m}$ be of the form $f_{\Sigma} = -\tilde{f}_{\Sigma}U$ with \tilde{f}_{Σ} a positive diffusion coefficient.

Theorem 5. Let Σ be a structured surface with surface energy ϕ . Let us assume

$$\frac{d}{dt} \int_{\mathfrak{b}_{\Sigma}} \mathcal{Q}_{\varepsilon} d^{3} \mathbf{X} + \int_{\partial \mathfrak{b}_{\Sigma}} \mathfrak{F}_{\varepsilon} \cdot \mathbf{n} d\mathcal{H}^{2} - \int_{\mathfrak{b}_{\Sigma}} \mathsf{m}_{\varepsilon} \left(\mathbf{w} \right) d^{3} \mathbf{X} - \int_{\mathfrak{b}_{\Sigma} \cap \Sigma} n_{\varepsilon} \left(\langle \mathbf{w} \rangle \right) d\mathcal{H}^{2} + \int_{\partial (\mathfrak{b}_{\Sigma} \cap \Sigma)} \mathfrak{X} \cdot \mathbf{n} dl + \int_{\mathfrak{b}_{\Sigma} \cap \Sigma} \mathbf{f}_{\Sigma} \cdot \mathfrak{w} d\mathcal{H}^{2} = 0, \qquad (96)$$

for any part \mathfrak{b}_{Σ} of \mathcal{B}_0 crossing Σ . If $\mathcal{L}_{\varepsilon}$ and ϕ are invariant with respect to $\hat{\mathbf{f}}_{s_1}^1, \mathbf{f}_{s_2}^2$, and G, covariant pointwise balances across Σ follow as in the list below.

1. The action of $\mathbf{f}_{s_2}^2$ alone implies the interfacial balance of standard interactions

$$[\mathbf{P}]\mathbf{m} + Div_{\Sigma} \mathbb{T} = -\rho_0 [\dot{\mathbf{x}}] U, \qquad (97)$$

where $\mathbb{T} = -\partial_{\mathbb{F}}\phi \in Hom(T_{\mathbf{X}}\Sigma, T_{\mathbf{x}}^*\mathcal{B})$ is the surface Piola-Kirchhoff stress.

2. The action of G alone implies the interfacial balance of substructural interactions

$$[\mathcal{S}]\mathbf{m} + Div_{\Sigma}\,\mathbb{S} - \mathfrak{z} - (1 - \varepsilon_2)\,\mathfrak{z}^v = -\varepsilon_1\bar{\rho}\,[\dot{\mathbf{w}}]\,U,\tag{98}$$

where $\mathbb{S} = -\partial_{\mathbb{N}}\phi \in Hom(T_{\mathbf{X}}\Sigma, T_{\mathbf{w}}^*\mathbb{V}_w)$ is the surface microstress and $\mathfrak{z} = \partial_{\langle \mathbf{w} \rangle}\phi \in T_{\langle \mathbf{w} \rangle}^*\mathbb{V}_w$ the surface self-force.

3. The action of $\hat{\mathbf{f}}_{s_1}^l$ alone implies the evolution equation of Σ along the normal \mathbf{m} , namely,

$$\mathbf{m} \cdot [\mathbb{P}] \,\mathbf{m} + \mathbb{C}_{\tan} \cdot \mathbf{L} + Div_{\Sigma} \,\mathbf{c} + (1 - \varepsilon_2) \,\langle \nabla \mathbf{w} \rangle^T \,\mathfrak{z}^v \cdot \mathbf{m} =$$
$$= \varepsilon_1 \bar{\rho} U \left[(\nabla \mathbf{w})^T \,\dot{\mathbf{w}} \right] \cdot \mathbf{m} + \frac{1}{2} \varepsilon_1 \bar{\rho} \left[|\dot{\mathbf{w}}|^2 \right] - \frac{1}{2} \rho_0 U^2 \left[|\mathbf{F}\mathbf{m}|^2 \right] + \tilde{f}_{\Sigma} U, \tag{99}$$

where

$$\mathbb{C}_{\text{tan}} = \phi \Pi - \mathbb{F}^T \mathbb{T} - \mathbb{N}^T \mathbb{S}$$
(100)

is a generalized version of the surface Eshelby stress accounting for phason surface interactions and

$$\mathbf{c} = -\partial_{\mathbf{m}}\phi - \mathbb{T}^T \langle \mathbf{F} \rangle \, \mathbf{m} - \mathbb{S}^T \langle \nabla \mathbf{w} \rangle \, \mathbf{m}$$
(101)

a surface shear.

Of course, the evaluation of the special cases corresponding to the combinations of the values of ε_1 and ε_2 is immediate and is left to the reader. In the case of quasicrystals,

the conservative part \mathfrak{z} of the surface self-force may disappear because ϕ may not depend on $\langle \mathbf{w} \rangle$.

An analogous theorem valid for abstract complex bodies can be found in [10], where only the conservative behavior is considered and dissipative effects are not accounted for, contrary to the theorem above. Moreover, though in [10] the morphological descriptors are elements of an abstract differentiable manifold \mathcal{M} (so one follows a unifying framework for models of condensed matter physics), the morphological descriptor map is continuous across Σ . Here, in contrast, we allow bounded jumps of w. When in multifield theories morphological descriptors are selected in a linear space, in fact, the related field can be considered discontinuous at Σ . On the contrary, when the manifold \mathcal{M} of substructural shapes does not coincide with a linear space, the jump of the morphological descriptor across Σ could not be defined. However, since \mathcal{M} has finite dimension, it can be embedded isometrically in an appropriate linear space, so that the definition of the jump could make sense, but the embedding itself becomes a prominent part of modeling. In fact, although the isometric embedding is preferable because it preserves the quadratic part of the substructural kinetic energy (if it exists as in IIC and IMC in pinning free states), such an embedding is not unique (as the non-isometric ones) and also not "rigid." Then, the selection of the appropriate embedding (if necessary in the case of abstract order parameters) is not simple and general criteria suggested by physical instances seems not to be available yet.

Proof. Conditions assuring the invariance of $\tilde{\phi}$ with respect to changes in observers and relabeling are given by $\frac{d}{ds_i}\phi|_{s_1=0,s_2=0,s_3=0}=0$, with i=1, 2, 3. They correspond to

$$\mathbb{F}^{T}\mathbb{T}\cdot\nabla_{\Sigma}\mathfrak{w} + \mathbb{N}^{T}\mathbb{S}\cdot\nabla_{\Sigma}\mathfrak{w} + \partial_{\mathbf{m}}\phi\cdot(\nabla\mathfrak{w})\mathbf{m} = 0, \qquad (102)$$

$$\mathbb{T} \cdot \nabla_{\Sigma} \mathbf{v} = 0, \tag{103}$$

$$\mathfrak{z} \cdot \xi_{\mathbb{V}_{\mathbf{W}}}\left(\langle \mathbf{w} \rangle\right) + \mathbb{S} \cdot \nabla_{\Sigma} \xi_{\mathbb{V}_{\mathbf{W}}}\left(\langle \mathbf{w} \rangle\right) = 0. \tag{104}$$

If we shrink \mathfrak{b}_{Σ} to $\mathfrak{b}_{\Sigma} \cap \Sigma$ uniformly in time, we get the pointwise balance

$$-\left[\mathcal{Q}_{\varepsilon}\right]U + \left[\mathfrak{F}_{\varepsilon}\right] \cdot \mathbf{m} + Div_{\Sigma} \mathfrak{X} - n_{\varepsilon}\left(\langle \mathbf{w} \rangle\right) + \mathbf{f}_{\Sigma} \cdot \mathfrak{w} = 0, \qquad (105)$$

as a consequence of the arbitrariness of \mathfrak{b}_{Σ} .

If \mathbf{f}^2 acts alone, then

$$\mathfrak{X} = \mathbb{T}^T \mathbf{v}, \qquad \mathcal{Q}_{\varepsilon} = \rho \dot{\mathbf{x}} \cdot \boldsymbol{v}, \qquad \mathfrak{F}_{\varepsilon} = -\mathbf{P}^T \mathbf{v}, \qquad (106)$$

so that, as a consequence of (103), $Div_{\Sigma} \mathfrak{X} = \mathbf{v} \cdot Div_{\Sigma} \mathbb{T}$. The arbitrariness of \mathbf{v} and its continuity across Σ implies (97) from (105).

If G acts alone, we get

$$\begin{aligned} \mathfrak{X} &= \mathbb{S}^T \xi_{\mathbb{V}_{\mathbf{W}}} \left(\langle \mathbf{w} \rangle \right), \qquad \mathcal{Q}_{\varepsilon} = \varepsilon_1 \bar{\rho} \dot{\mathbf{w}} \cdot \xi_{\mathbb{V}_{\mathbf{W}}} \left(\langle \mathbf{w} \rangle \right), \\ \mathfrak{F}_{\varepsilon} &= -\mathcal{S}^T \xi_{\mathbb{V}_{\mathbf{W}}} \left(\langle \mathbf{w} \rangle \right), \qquad n_{\varepsilon} \left(\langle \mathbf{w} \rangle \right) = (1 - \varepsilon_2) \mathfrak{z}^{\upsilon} \cdot \xi_{\mathbb{V}_{\mathbf{W}}} \left(\langle \mathbf{w} \rangle \right), \end{aligned} \tag{107}$$

and, from (104),

$$Div_{\Sigma} \mathfrak{X} = \xi_{\mathbb{V}_{\mathbf{w}}} \left(\langle \mathbf{w} \rangle \right) \cdot \left(Div_{\Sigma} \, \mathbb{S} - \mathfrak{z} \right). \tag{108}$$

Then, from (105) we obtain (98) thanks to the arbitrariness of the element ξ selected in the Lie algebra of *G*.

If $\hat{\mathbf{f}}^1$ acts alone, then

$$\mathcal{Q}_{\varepsilon} = -\rho_0 \mathbf{F}^T \dot{\mathbf{x}} \cdot \boldsymbol{\mathfrak{w}} - \varepsilon_1 \bar{\rho} \left(\nabla \mathbf{w} \right)^T \dot{\mathbf{w}} \cdot \boldsymbol{\mathfrak{w}}, \tag{109}$$

$$\mathfrak{F}_{\varepsilon} = \left(\left(\frac{1}{2} \rho_0 \left| \dot{\mathbf{x}} \right|^2 + \frac{1}{2} \varepsilon_1 \bar{\rho} \left| \dot{\mathbf{w}} \right|^2 \right) \mathbf{I} - \mathbb{P} \right)^T \mathfrak{w} + \rho_0 w \left(\mathbf{x} \right) \mathfrak{w}, \tag{110}$$

$$\mathfrak{X} = -\mathbb{C}_{\tan}^T \mathfrak{w} - \mathfrak{c} \mathbf{V}_m, \qquad (111)$$

$$n_{\varepsilon}\left(\langle \mathbf{w} \rangle\right) = -\left(1 - \varepsilon_{2}\right) \left\langle \nabla \mathbf{w} \right\rangle^{T} \mathfrak{z}^{v} \cdot \mathfrak{w}, \qquad (112)$$

with \mathbb{C}_{tan} and \mathfrak{c} defined respectively by (100) and (101) and $\mathbf{v}_m = \mathfrak{w} \cdot \mathbf{m}$.

Terms of equation (105) then become in this case

$$-[\mathcal{Q}_{\varepsilon}]U + [\mathfrak{F}_{\varepsilon}] \cdot \mathbf{m} = \rho_{0}[\mathbf{F}^{T}\dot{\mathbf{x}}]U \cdot \mathfrak{w} + \varepsilon_{1}\bar{\rho}[(\nabla \mathbf{w})^{T}\dot{\mathbf{w}}]U \cdot \mathfrak{w} + \frac{1}{2}\rho_{0}[|\dot{\mathbf{x}}|^{2}]\mathfrak{w} \cdot \mathbf{m} + \frac{1}{2}\varepsilon_{1}\bar{\rho}[|\dot{\mathbf{w}}|^{2}]\mathfrak{w} \cdot \mathbf{m} - [\mathbb{P}]\mathfrak{w} \cdot \mathbf{m},$$
(113)

$$Div_{\Sigma} \left(\mathbb{C}_{\tan}^{T} \mathfrak{w} + \mathfrak{c} \mathsf{V}_{m} \right) = \mathfrak{w} \cdot \left(Div_{\Sigma} \mathbb{C}_{\tan} + \left(Div_{\Sigma} \mathfrak{c} \right) \mathfrak{m} \right),$$
(114)

where the second equation is a consequence of (102), the circumstance that

$$(\mathbf{I} - \mathbf{m} \otimes \mathbf{m}) \cdot \nabla_{\Sigma} \mathfrak{w} = ((\nabla \mathfrak{w}) \, \mathbf{m}) \cdot \mathbf{m}, \tag{115}$$

since \mathfrak{w} is isochoric, and properties 3 and 4 of the definition of the relabeling $\hat{\mathbf{f}}^{I}$ of \mathcal{B}_{0} including Σ .

By inserting (113) and (114) into (105), the arbitrariness of w implies

$$\rho_{0}[\mathbf{F}^{T}\dot{\mathbf{x}}]U + \varepsilon_{1}\bar{\rho}[(\nabla\mathbf{w})^{T}\dot{\mathbf{w}}]U + \frac{1}{2}\rho_{0}[|\dot{\mathbf{x}}|^{2}]\mathbf{m} + (1 - \varepsilon_{2})\langle\nabla\mathbf{w}\rangle^{T}\mathfrak{z}^{\upsilon} + \frac{1}{2}\varepsilon_{1}\bar{\rho}[|\dot{\mathbf{w}}|^{2}]\mathbf{m} = [\mathbb{P}^{T}]\mathbf{m} + Div_{\Sigma}\mathbb{C}_{\mathrm{tan}} + (Div_{\Sigma}\mathfrak{c})\mathbf{m} + \mathbf{f}_{\Sigma}\cdot\mathfrak{w}, \qquad (116)$$

and we shall evaluate the component along \mathbf{m} of (116).

By indicating with $\bar{\mathbf{v}}$ the averaged velocity $\bar{\mathbf{v}} = \langle \dot{\mathbf{x}} \rangle + U \langle \mathbf{F} \rangle \mathbf{m}$ and using the relation $[\dot{\mathbf{x}}] = -U[\mathbf{F}]\mathbf{m}$ mentioned previously, we then get

$$\rho_0[\mathbf{F}^T \dot{\mathbf{x}}] U \cdot \mathbf{m} = -\frac{1}{2} [\rho_0 |\dot{\mathbf{x}} - \bar{v}|^2] = \rho_0[\dot{\mathbf{x}}] \cdot \bar{\mathbf{v}} - \rho_0[|\dot{\mathbf{x}}|^2], \qquad (117)$$

where $\frac{1}{2} = \rho_0 |\dot{\mathbf{x}} - \bar{v}|^2$ is the relative kinetic energy referred to Σ . We also get

$$\frac{1}{2}\rho_0[|\dot{\mathbf{x}}|^2] = -\rho_0[\dot{\mathbf{x}}] \cdot \bar{\mathbf{v}} + \frac{1}{2}\rho_0 U^2[|\mathbf{Fm}|^2], \qquad (118)$$

by using once more $[\dot{\mathbf{x}}] = -U[\mathbf{F}]\mathbf{m}$ and the definition of $\bar{\mathbf{v}}$. By evaluating the normal component of (116), using (117), (118), and taking into account that

$$\mathbf{m} \cdot Div_{\Sigma} \,\mathbb{C}_{\mathrm{tan}} = \mathbb{C}_{\mathrm{tan}} \cdot \mathsf{L},\tag{119}$$

as it is simple to verify (see Lemma 2 in [10]), we get (99), and the final part of the theorem follows. $\hfill \Box$

Corollary 6. In absence of surface energy and surface friction, interfacial balances become respectively

$$[\mathbf{P}]\,\mathbf{m} = -\rho_0\,[\dot{\mathbf{x}}]\,U,\tag{120}$$

$$[\mathcal{S}]\mathbf{m} = -\varepsilon_1 \bar{\rho} \,[\dot{\mathbf{w}}] \, U, \tag{121}$$

$$\mathbf{m} \cdot \left[\mathbb{P}\right] \mathbf{m} = \varepsilon_1 \bar{\rho} U \left[(\nabla \mathbf{w})^T \, \dot{\mathbf{w}} \right] \cdot \mathbf{m} + \frac{1}{2} \varepsilon_1 \bar{\rho} \left[|\dot{\mathbf{w}}|^2 \right] - \frac{1}{2} \rho_0 U^2 \left[|\mathbf{Fm}|^2 \right] + \tilde{f}_{\Sigma} U. \quad (122)$$

8. SO(3) Invariance and the Nature of the Balance of Phason Interactions

In deriving the balance (33), we have mixed the representation of phason interactions (phason stress and phason self-force) and their constitutive structure declared through the derivatives of the Lagrangian with respect to $\nabla \mathbf{w}$ and \mathbf{w} respectively, together with (8). A question is whether the pointwise balance of phason interactions holds before inserting constitutive laws. Another connected question is whether an integral (global) version of the pointwise balance of phason interactions can be postulated a priori as a balance of phason-momentum.

• The answer to the first question is affirmative: The balance of phason interactions holds in the form

$$Div\,\mathcal{S} - \bar{\mathbf{z}} + \boldsymbol{\beta} = 0,\tag{123}$$

independently of constitutive laws, where β represents possible phason inertia and the self-force \bar{z} includes both conservative and dissipative components in an additive way (as it will be clear below).

• As regards the second question, though an integral version of (123) can be postulated in principle *because* \mathbb{V}_w is a linear space, it is *not* necessary because just the integral balance of standard forces and a nonstandard balance of moments suffices to get pointwise balances.

To prove previous statements, we leave constitutive laws out of consideration and try to represent interactions only in their purely geometric nature, i.e. the one of objects power conjugated with the rates of the descriptors of the morphology of the body, namely phonon and phason degrees of freedom.

Let b be any part of \mathcal{B}_0 , i.e., any subset of \mathcal{B}_0 with nonnull volume measure and the same regularity properties of \mathcal{B}_0 . We presume that b interacts with the rest of the body and the external environment by means of interactions of bulk and contact nature, the latter exerted through the boundary ∂b . The external power $\mathcal{P}_b^{ext}(\dot{\mathbf{x}}, \dot{w})$ of all external actions over b, a linear functional over the space of rates $\dot{\mathbf{x}}$ and $\dot{\mathbf{w}}$, is then given by

$$\mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{\mathbf{x}},\dot{w}\right) = \int_{\mathfrak{b}} \left(\bar{\mathbf{b}}\cdot\dot{\mathbf{x}} + \beta\cdot\dot{\mathbf{w}}\right) d^{3}\mathbf{X} + \int_{\partial\mathfrak{b}} \left(\mathbf{P}\mathbf{n}\cdot\dot{\mathbf{x}} + \mathcal{S}\mathbf{n}\cdot\dot{\mathbf{w}}\right) d\mathfrak{H}^{2}.$$
 (124)

Here, $\mathbf{\bar{b}}$ represents standard bulk forces and is decomposed as $\mathbf{\bar{b}} = \mathbf{b} + \mathbf{b}^{in}$, where **b** is the objective part coincident with the analogous **b** in Corollary 1, and \mathbf{b}^{in} is of pure inertial phonon nature. β is of pure inertial phason nature (if phason inertia exists, as

in IIC and IMC in pinning free states), while **P** and *S* are respectively the first Piola-Kirchhoff stress and the phason stress, as in previous sections. **Pn** represents the tractiondeveloping power in the relative change of place of neighboring material elements at the boundary ∂b , by imagining the phason activity frozen. *Sn* pictures interactions developed across the boundary ∂b between neighboring material elements which do not change place but display different phason activity. As pointed out above, at each **X** we get $\mathbf{P} \in Hom(T_{\mathbf{X}}^*\mathcal{B}_0, T_{\mathbf{x}}^*\mathcal{B})$ and $S \in Hom(T_{\mathbf{X}}^*\mathcal{B}_0, T_{\mathbf{w}}^*\mathbb{V}_w)$. Over $\partial \mathfrak{b}$ we indicate by $d\mathfrak{H}^2$ the relevant two-dimensional Hausdorff measure.

We now require the *invariance* of \mathcal{P}_{b}^{ext} ($\dot{\mathbf{x}}$, $\dot{\mathbf{w}}$) with respect to (classical) changes in observers ruled by *SO* (3). For such changes, the time-parametrized family of automorphisms acting on the ambient space \mathcal{E}^{3} is the one of isometries so that, as usual, if $\dot{\mathbf{x}}^{*}$ is the value of the velocity $\dot{\mathbf{x}}$ after the change in observer, we get

$$\dot{\mathbf{x}}^* = \mathbf{c}\left(t\right) + \dot{\mathbf{q}}\left(t\right) \times \left(\mathbf{x} - \mathbf{x}_0\right) + \dot{\mathbf{x}},\tag{125}$$

where $\mathbf{c}(t)$ is the translational velocity, constant in space, \mathbf{x}_0 a point chosen arbitrarily and $\dot{\mathbf{q}} \times \in \mathfrak{so}(3)$ at each *t*. Moreover, still for such changes in observers, *SO*(3) itself acts also over \mathbb{V}_w , and if we indicate with $\dot{\mathbf{w}}^*$ the rate $\dot{\mathbf{w}}$ measured after such a change, we get

$$\dot{\mathbf{w}}^* = \dot{\mathbf{w}} + \dot{\mathbf{q}}\left(t\right) \times \mathbf{w}.$$
(126)

Then, the requirement of invariance is

$$\mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{\mathbf{x}}^{*},\dot{\mathbf{w}}^{*}\right) = \mathcal{P}_{\mathfrak{b}}^{ext}\left(\dot{\mathbf{x}},\dot{\mathbf{w}}\right),\tag{127}$$

for *any* choice of translational \mathbf{c} and rotational $\dot{\mathbf{q}}$ velocities and for any part \mathbf{b} (see [24] for a more general setting involving abstract morphological descriptors).

The arbitrariness of **c** and $\dot{\mathbf{q}}$ and their independence of space imply from (127) the integral balances

$$\int_{\mathfrak{b}} \bar{\mathbf{b}} d^3 \mathbf{X} + \int_{\partial \mathfrak{b}} \mathbf{Pn} d\mathfrak{H}^2 = 0, \qquad (128)$$

$$\int_{\mathfrak{b}} \left((\mathbf{x} - \mathbf{x}_0) \times \bar{\mathbf{b}} + \mathbf{w} \times \boldsymbol{\beta} \right) d^3 \mathbf{X} + \int_{\partial \mathfrak{b}} \left((\mathbf{x} - \mathbf{x}_0) \times \mathbf{P} \mathbf{n} + \mathbf{w} \times \boldsymbol{\mathcal{S}} \mathbf{n} \right) d\mathfrak{H}^2 = 0, \quad (129)$$

which are respectively the standard integral balance of forces and a nonstandard (due to the presence of phason interactions) integral balance of moments. They are the sole global conservation laws associated with the Killing fields of the metric in the ambient space.

The arbitrariness of b implies

$$\mathbf{b} + Div\,\mathbf{P} = \mathbf{0},\tag{130}$$

from (128), and

$$\mathbf{ePF}^{T} = \mathbf{w} \times (\boldsymbol{\beta} + Div\,\mathcal{S}) + (\nabla \mathbf{w})^{T}\,\mathcal{S},\tag{131}$$

from (129), with e Ricci's alternating symbol.

From (131) we get two pieces of information:

- 1. At each $\mathbf{X} \in \mathcal{B}_0$, the term $\mathbf{ePF}^T (\nabla \mathbf{w})^T \mathcal{S}$ is given by the cross product between \mathbf{w} and an element of $T^*_{\mathbf{w}} \mathbb{V}_w \simeq \mathbb{R}^3$ that we indicate by $\bar{\mathbf{z}}$;
- 2. $\bar{\mathbf{z}}$ is just equal to $Div S \bar{\rho} \ddot{\mathbf{w}}$, so that we get (123).

The inertial component of \mathbf{b} , namely \mathbf{b}^{in} , and the explicit expression of $\boldsymbol{\beta}$ can be identified by requiring that their power is the opposite of the rate of the kinetic energy, i.e.,

$$\frac{d}{dt} \{ \text{kinetic energy in } \mathfrak{b} \} - \int_{\mathfrak{b}} \left(\mathbf{b}^{in} \cdot \dot{\mathbf{x}} + \beta \cdot \dot{\mathbf{w}} \right) d^3 \mathbf{X} = 0,$$
(132)

for any choice of b and of the velocity fields. When soundlike modes of phason nature appear (this is the case of IIC and IMC), the kinetic energy in b is given by $\frac{1}{2} \int_{b} (\rho_0 |\dot{\mathbf{x}}|^2 + \varepsilon_1 \bar{\rho} |\dot{\mathbf{w}}|^2) d^3 \mathbf{X}$, as in IIC and IMC, the arbitrariness of b and of the velocity fields implies

$$\mathbf{b}^{in} = -\rho_0 \ddot{\mathbf{x}}, \qquad \boldsymbol{\beta} = -\varepsilon_1 \bar{\rho} \ddot{\mathbf{w}}. \tag{133}$$

In this way (130) reduces formally to (32).

Moreover, we may assume that \bar{z} admits an additive decomposition in its conservative (z) and nonconservative (z^{v}) parts as

$$\mathbf{z} = \bar{\mathbf{z}} + \mathbf{z}^{\nu},\tag{134}$$

with \mathbf{z}^{v} purely dissipative in the sense defined in Section 3, so that we get (8).

Remark 9. In summary, when we represent interactions due to phason activity in quasiperiodic crystalline structures, an internal self-force appears a priori just as a consequence of requirements of SO(3) invariance of the external power. Constitutive laws render explicit its structure as a function of state, and we find that the conservative part of z disappears for quasicrystals because the relevant elastic energy does not depend on w while its dissipative part plays a role.

9. Concluding Remarks

Quasi-periodic alloys are a paradigmatic example of complex bodies: bodies for which microstructural (or, more generally, substructural) changes prominently influence the gross mechanical behavior in a way in which the conjugated interactions cannot be neglected. For IIC and IMC these changes are relative shifts between atomic lattices with incommensurate period or "modulations" of standard periodic crystalline lattices that become quasi-periodic. For quasicrystals, substructural changes are collective atomic modes and tunneling of atoms below energetic barriers that generate worms (topological alterations with respect to the prevailing crystal symmetry which do not fit the standard crystallographic classification). These changes are referred to as "phason activity" in this paper. Information about them in the geometrical description of the body is carried by a morphological descriptor of the substructural changes "within" each material element

(crystalline patch). The descriptor is a vector **w** prompted by the Fourier representation of the mass density on quasi-periodic lattices (as specified in the Introduction).

Differences between incommensurate structures (the ones of IIC and IMC) and quasicrystals are of a constitutive nature; moreover, phason kinetic energy can be attributed to both IIC and IMC, while it is not present in quasicrystals.

Phason activity alters the energetic landscape of the body from place to place so that substructural interactions appear and are power-conjugated with phason activity itself. These interactions satisfy an appropriate pointwise balance in the bulk material: a balance covariant in the sense that it derives from a requirement of invariance under changes in observers governed by the action of an arbitrary Lie group G on the space of ws. When G reduces to SO(3), one recovers classical invariance with respect to changes in observers differing by rigid body motions. Our invariance requirement is stronger than this classical one, and Corollary 1 shows that the balance of substructural interactions is, in a certain sense, more fundamental than expected. In particular, the arbitrariness of G renders it unimportant to specify how w transforms under changes in spatial coordinates. The proof of the covariance of the balance of phason interactions is based on a Noetherlike theorem (Theorem 1). Such a theorem is not derived in the standard conservative setting and, in contrast to a similar proposal in the general setting of multifield theories for the mechanics of complex bodies, it accounts for nonconservative effects due to the presence of phason friction. The presence of substructural interactions also leads to nonsymmetric Cauchy stresses as pointed out by the requirement of SO(3) invariance (Corollary 2).

Invariance with respect to relabeling is also assured for a balance of configurational forces acting on nonevolving bulk defects, as shown in Corollary 3. An extended version of the Eshelby tensor is involved: It accounts for the influence of phason activity on possible defects (their motion and/or their equilibrium) and is generated by the variation of the energy with respect to variations of the material metric, the latter variations induced by the defects themselves (Theorem 3).

When deformation processes are faster than the "activation time" of phason friction in quasicrystals, the balance equations at equilibrium admit universal solutions (i.e., solutions independent of constitutive laws) that describe both affine macroscopic deformations and affine phason activity. However, in contrast to the proof of the analogous result on universal solutions in standard nonlinear elasticity of simple bodies, here the derivatives of the first Piola-Kirchhoff stress and the phason stress must satisfy an additional pointwise algebraic condition, a circumstance that "diminishes" in a certain sense the generality of the result.

It is rather immediate to show how existing linear theories on the mechanics of quasiperiodic alloys, and quasicrystals in particular, are contained in the general nonlinear theory proposed here. Implications of the present multifield modeling are illustrated by an application of the linearized theory to quasicrystals, in particular to *AlPbMn*based alloys (Section 6): The resulting localization and quasi-phasonic waves cannot be obtained from standard linear elasticity.

Wall defects may occur and possibly evolve in quasi-periodic alloys. They are represented by surfaces across which some fields suffer bounded discontinuities. Surface energy is accounted for: Its presence models the circumstance that wall defects are often thin layers capable of sustaining surface stresses. An evolution equation can be derived

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(Theorem 5) that accounts for the influence of phason activity and describes a generalized version of the motion-by-curvature. Interfacial pointwise balances of standard and phason interactions can also be derived in a covariant manner (Theorem 5) from an integral balance involving the relative power densities that appear in Theorem 1, their surface counterparts and the power of the force irreversibly driving wall defects. Such an integral balance is also the source of the pointwise evolution equation of the wall defects, an equation which is materially covariant, in the sense that it accrues from an invariance request with respect to relabeling.

By exploiting SO(3) invariance of the power of external actions over an arbitrary part of the body, one gets the existence of the internal self-force (which, in contrast, is commonly postulated), independent of constitutive laws that specify it subsequently.

In describing the mechanics of quasi-periodic alloys, as in all cases of complex bodies, one faces phenomena occurring at different scales: here, macroscopic and atomic. The multifield modeling of quasi-periodic alloys proposed here (as in all cases in which one adopts a multifield point of view for some special class of complex bodies) allows one to represent everything at a unique macroscopic scale.

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