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A note on the thermo-mechanics of elastic quasi-crystals

G rard A. Maugin

Abstract In recent years, many papers have been published concerning the elasticity of quasi-crystals. The present study has for main purpose to replace the proposed formulations into the framework of the modern thermo-mechanics of continua. Two types of modelling are envisaged in small deformations, those inspired by the physical descriptions proposed by Bak on the one hand and by Lubensky and co-workers on the other. While the first one fits well in a traditional variational formulation, the second one seems to be best accommodated in the frame of the thermo-mechanics of internal variables of state, the newly introduced “phason” field being then interpreted as such a vector variable. The inclusion of these two models in the theory of configurational forces—useful for the study of the expansion of defects frequent in such crystals—and the possibilities of including the effects of nonlinear elasticity and plasticity are briefly discussed. Important symmetry conditions are however left aside.

Keywords Quasi-crystals · Elasticity · Phonon · Phason · Thermo-mechanics · Internal variables · Configurational forces · Nonlinearity

1 Introduction

Without entering the technicalities of condensed matter physics for which we are not expert, we note that *quasi-crystals* experimentally discovered in certain alloys in 1982 by D. Shechtman (Nobel Prize in Chemistry 2011) and with an initial symmetry theory proposed in 1984 (see Lubensky [1], Fan [2], Trebin [3] for the history and main structural and physical properties) present a challenge for their modelling as deformable continua. It is acknowledged that they present some aperiodicity (or quasi-periodicity along certain directions or in planes) which is their main characteristic symmetry property. This allows for the acceptance of symmetries (e.g. fivefold orientational symmetry) that were heretofore forbidden but are now revealed in diffraction experiments for certain alloys. Furthermore, their strange symmetry behaviour is macroscopically represented by the co-existence of two elementary excitations (in the sense of Lev D. Landau), a rather classical one, known as *phonons* (the typical vibrations of regular periodic crystal lattices) in the physical so-called parallel space and a new internal one in the so-called orthogonal space referred to as *phason* that corresponds to a relative motion of the constituent density waves of condensed matter physics (in other words, the internal rearrangements of an environment—cf. G hler et al. [4]). Phenomenologically, one displacement is associated with each of these, but whereas one interpretation favours a vision somewhat parallel for the two displacements with particular structural disorder or structure fluctuations associated with the phasons (here referring to Bak’s vision), another interpretation sees the phasons as diffusive with large diffusive time (Lubensky et al). Here, we examine these

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two possibilities from the point of view of the phenomenological (continuum) thermo-mechanics of continua, being also aware of the importance of the role played by defects and some nonlinearities in such crystals (as emphasized in the book of Fan [2]). As a consequence we also examine the formulation of configurational forces and the associated conservation (or non-conservation) laws that accompany the more standard field equations.¹ This is achieved in the spirit of our recent book [5].

The paper is organized as follows. After this introduction, the general field equations pertaining to the two modelling schemes are recalled in the first paragraph of Sect. 2. The possibility to accommodate the second scheme by means of the thermodynamics of internal variables of state is exposed in Sect. 2.2. The construction of the main associated conservation law (the so-called wave momentum) is given in Sect. 3 for the two schemes together with the expression of the driving force on defects. Section 4 provides some remarks on the possible nonlinearity of the mechanical response. A brief conclusion is drawn in Sect. 5. Exceptionally, we use only a Cartesian tensor notation (with its usual conventions) that is accessible to all, engineers and physicists.

2 General field equations

Here, we consider the basic continuum field equations that are supposed to govern the elasticity of quasi-crystals. We are interested in the *dynamics* of these crystals so that inertia and evolution in time are taken into account, depending on the selected model. Two such models will be referred to as the “Bak” (inspired) model and the “Lubensky” (inspired) model according to the main authors of these two possibilities ([6–9] in the first case) and Lubensky et al. [1, 10, 11] in the second case).

2.1 The “Bak” dynamic model

In this case, the equations of linear momentum associated with both phonons and phasons have a standard form with inertial terms, i.e. in Cartesian tensor notation (cf. Fan [2], p. 39; $i, j = 1, 2, 3$ with Einstein summation convention on dummy indices),

$$\frac{\partial}{\partial x_j} \sigma_{ji} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2} \text{ (phonons)}, \quad (1)$$

$$\frac{\partial}{\partial x_j} H_{ji} + g_i = \rho \frac{\partial^2 w_i}{\partial t^2} \text{ (phasons)}, \quad (2)$$

where σ_{ji} is the *symmetric* stress tensor for “phonons”, H_{ji} is the generally non-symmetric stress tensor for “phasons”, f_i and g_i are the corresponding (if any) external forces per unit volume, u_i is the standard elastic displacement vector, w_i is the “phason” displacement vector, and ρ is the matter density. In the absence of dissipative effects, the two stresses are derived from a volume energy density $W(e_{ij}, w_{ij})$ by

$$\sigma_{ji} = \frac{\partial W}{\partial e_{ij}}, \quad H_{ji} = \frac{\partial W}{\partial w_{ij}}, \quad (3)$$

where

$$e_{ij} = e_{(i,j)} := \frac{1}{2} (u_{i,j} + u_{j,i}), \quad w_{ij} := w_{i,j}, \quad (4)$$

where a partial space derivative is denoted by a comma followed by an index. Note here that w_{ij} is not reduced to its symmetric part since the “phason” field gradient is not subjected to rotational invariance, having in fact two indices that refer to directions in two different spaces (the internal or orthogonal space and the physical space).

In this framework, the global medium may be viewed as the interaction—via the strain energy function—between two continua that are essentially elastic (cf. Levine et al. [11]). Only the peculiarity of the second definition in (4)—cf. the already noted absence of symmetrisation—and the application of material symmetry

¹ The study reported in this work was suggested to the author while being the editor and referee of several papers on the elasticity of quasi-crystals. It results from a specific effort from the author to comprehend the basis elements of this elasticity, as in particular exposed in a recent book by Fan [2], and to replace its two basic formulations in a more familiar thermo-mechanical background as accepted in modern continuum mechanics.

conditions will clearly distinguish the behaviour of one component from the other. The theory can be deduced from a standard Lagrangian–Hamiltonian variational principle fundamentally based on the expression (T is a time interval, and B stands for a regular three-dimensional body)

$$\delta \int_T \int_B L d^3x dt = 0, L = K - W, \quad (5)$$

in the absence of external body forces, and

$$K = \frac{1}{2} \rho \dot{u}_i \dot{u}_i + \frac{1}{2} \rho \dot{w}_i \dot{w}_i, \quad (6)$$

where a superimposed dot denotes the partial time derivative.

2.2 The “Lubensky” dynamic model

In this case, Eqs. (1) and (2) are replaced by the equations

$$\frac{\partial}{\partial x_j} \sigma_{ji} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2} (\text{phonons}), \quad (7)$$

$$\frac{\partial}{\partial x_j} H_{ji} + g_i = \kappa \frac{\partial w_i}{\partial t} (\text{phasons}), \quad (8)$$

where the stress tensors are still given by constitutive equations (3) with definitions (4) and κ is the reciprocal of the kinetic coefficient for the phason field. The system (7) and (8) couples a wave equation with an evolution–diffusion equation so that we can expect a dynamic response quite different from that derivable from the set (1) and (2). Moreover, system (7) and (8) is no longer derivable from a Lagrangian–Hamiltonian variational formulation. Another type of approach involving irreversible thermodynamics is necessary to justify this system on a continuum basis. We believe that this can be formally accommodated within the thermodynamics of continua which involves the so-called internal variables of state, the phason displacement being here a vectorial internal variable of state (*not* an internal degree of freedom). This thermodynamics for short *T.I.V* that represents the slightest deviation from the classical theory of irreversible processes is documented in a book [12]. The related “internal” variables are not directly controllable by external forces (thus g_i should vanish), and it simply contributes to the expression of the free energy of the system, while its evolution is governed by the second law of thermodynamics. To formulate this approach, one needs to return to the general equations of a continuum with a special caution concerning the entropy flux. A priori no internal variable of state shows up in the basic equations. We consider only small deformations and an obvious notation. We have the following local equations:

- the local balance of linear and angular momenta:

$$\frac{\partial}{\partial x_j} \sigma_{ji} + f_i = \rho \frac{\partial^2 u_i}{\partial t^2}, \sigma_{ij} = \sigma_{ij}; \quad (9)$$

- the first law of thermodynamics:

$$\frac{\partial}{\partial t} (K + E) - \frac{\partial}{\partial x_j} (\sigma_{ji} \dot{u}_i - q_j) = \rho h; \quad (10)$$

- the second law of thermodynamics:

$$\frac{\partial}{\partial t} S \geq \frac{\partial s_i}{\partial x_i} - \rho \frac{h}{\theta}; \quad (11)$$

where E is the internal energy per unit volume, q_j and s_i stand for the heat flux vector and entropy flux vector, respectively, and S is the entropy per unit volume. Finally, θ is the thermodynamic temperature ($\theta > 0$, $\inf \theta = 0$). Here,

$$K = \frac{1}{2} \rho \dot{u}_i \dot{u}_i \quad (12)$$

only, and

$$s_i = k_i + \frac{q_i}{\theta}. \quad (13)$$

Vector k_i is called the *extra* entropy flux; it vanishes in most continuum theories save in the presence of diffusive processes (cf. Maugin [12]), which will be the case in this paragraph.

Introducing the free energy per unit volume W by $W = E - \theta S$, and accounting for (9), (12) and (13), combination of (10) and (11) yields the following *Clausius–Duhem inequality*:

$$-(\dot{W} + S\dot{\theta}) + \sigma_{ji} \dot{e}_{ij} + (\theta k_i)_{,i} - s_i \theta_{,i} \geq 0. \quad (14)$$

Now, we introduce the dependence of the free energy on *both* observable and internal variables of state by considering the function

$$W = \bar{W}(e_{ij}, w_i, w_{i,j}, \theta). \quad (15)$$

Substituting from this into (14), we obtain for the latter *sufficient* conditions for its satisfaction as

$$\sigma_{ji} = \frac{\partial \bar{W}}{\partial e_{ij}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \quad (16)$$

and

$$A_i \dot{w}_i - s_i \theta_{,i} \geq 0, \quad (17)$$

with

$$A_i = -\frac{\delta \bar{W}}{\delta w_i} = -\left(\frac{\partial \bar{W}}{\partial w_i} - \frac{\partial}{\partial x_j} \frac{\partial \bar{W}}{\partial w_{i,j}} \right), \quad k_i = -\frac{1}{\theta} \frac{\partial \bar{W}}{\partial w_{i,j}} \dot{w}_j \quad (18)$$

A frequent working hypothesis in *T.I.V* is to split the remaining dissipation inequality (17) in two parts related to heat conduction and entropy production due to the internal variable, yielding thus

$$s_i \theta_{,i} \leq 0, \quad A_i \dot{w}_i \geq 0. \quad (19)$$

The first of these will eventually yield Fourier’s law of heat conduction (note that the entropy flux always is the thermodynamic conjugate of the temperature gradient, whether k_i vanishes or not). As to the second, a simple evolution–diffusion model is obtained by taking W independent of w_i but quadratic in the gradient of this variable and assuming that A_i is directly proportional to \dot{w}_i —and thus guaranteeing the satisfaction of the second of (19). We obtain thus

$$\frac{\partial H_{ji}}{\partial x_j} = \kappa \frac{\partial w_i}{\partial t}, \quad H_{ji} \equiv \frac{\partial \bar{W}}{\partial w_{i,j}}, \quad \kappa \geq 0. \quad (20)$$

We have thus formally—but within thermodynamical admissibility—obtained the basic equations of the thermo-elasticity of quasi-crystals in the “Lubensky” format of the so-called *elasto-hydrodynamics* of such materials [13]. This can obviously be discussed since this is purely phenomenological and the true “quasi-crystal” nature of the studied material will be made evident only after specifying W and imposing appropriate symmetry conditions.

The above type of approach in *T.I.V* with a non-standard entropy flux and a possible diffusion of an internal variable of state was introduced in Maugin [14] in an abstract form. Of course the reasoning yielding the first of (20) from the second of (19) reminds us of the Landau–Ginzburg methodology in the physics of phase transformations.

3 Conservation laws and configurational forces in elastic quasi-crystals

As we know now (cf. the general overview in Ref. [5]), a comprehensive approach to the theory of structural defects and the driving forces acting on such defects calls for the due consideration of the so-called “conservation laws”—not to be mistaken for the standard balance laws of continuum mechanics—that pertain to the invariance of the whole physical under examination. For variationally derived field equations, these conservation laws are obtained by a strict application of a celebrated theorem due to Noether [15]. We shall not give the detail of this application which is canonical (but see below the notion of Noether’s identity) in the case of the coupled field equations (1) and (2) derived from the principle (5). Suffice it to notice that for invariance of the whole physical system under translations in material configuration space accounting for the absence of material inhomogeneities, the following conservation of “wave momentum” is obtained in the absence of external forces:

$$(\text{WM})_i := \frac{\partial}{\partial t} p_i^W - \frac{\partial}{\partial x_j} b_{ji} = 0, \quad (21)$$

wherein

$$p_i^W = p_i^u + p_i^w = -\rho (\dot{u}_k u_{k,i} + \dot{w}_k w_{k,i}) \quad (22)$$

and

$$b_{ji} = - (L \delta_{ji} + \sigma_{jk} u_{k,i} + H_{jk} w_{k,i}) \quad (23)$$

may be referred to as the total “wave momentum” and Eshelby stress tensor, respectively. The latter is not symmetric in general. Equation (21) is a direct consequence of Noether’s identity.

If we use the following short-hand notation:

$$(\text{EL})_k^u := \frac{\partial}{\partial t} \rho \dot{u}_k^- \frac{\partial}{\partial x_j} \sigma_{jk} = 0, \quad (\text{EL})_k^w := \frac{\partial}{\partial t} \rho \dot{w}_k^- \frac{\partial}{\partial x_j} H_{jk} = 0, \quad (24)$$

then the corresponding Noether’s identity reads

$$(\text{EL})_k^u u_{k,i} + (\text{EL})_k^w w_{k,i} + (\text{WM})_i = 0, \quad (25)$$

from which (21) follows at once.

In the case of the system (7) and (8) that is not derivable from a variational principle, a different strategy must be implemented. But a hint is provided by the identity (25) that we can mimic by applying $u_{i,k}$ to (7) and $w_{i,k}$ to (8) both with vanishing external forces—and summing the two on account of a free energy of the functional form $W = \overline{W}(e_{ij}, w_{i,j}, \theta)$. This manoeuvre results in the following equation of “wave momentum”:

$$(\text{WM})_i := \frac{\partial}{\partial t} p_i^W - \frac{\partial}{\partial x_j} b_{ji} - f_i^{th} - f_i^w = 0, \quad (26)$$

wherein b_{ji} is formally left unchanged but with the following reductions,

$$p_i^W = p_i^u = -\rho \dot{u}_k u_{k,j}, \quad K = \frac{1}{2} \rho \dot{u}_i \dot{u}_i, \quad (27)$$

while there appears as source terms forces of pseudo-inhomogeneity due to the two present dissipative processes, explicitly,

$$f_i^{th} := S \theta_{,i}, \quad f_i^w = (\kappa/\rho) p_i^w, \quad (28)$$

where p_i^w would be a wave momentum associated with phasons if they were of the propagative type [compare to the second contribution within parentheses in (22)]:

$$p_i^w = -\rho \dot{w}_k w_{k,i}. \quad (29)$$

The source term f_i^{th} of thermal origin is known in standard thermo-elasticity since 1978 in small strains (H.D. Bui) and more generally since 1995 (See [5], Chapter 5). The source term f_i^w due to the diffusion of the phason field reminds us of a source term exhibited (cf. Fomethé and Maugin [16]) in the magnetoelasticity of elastic ferromagnets that couples an essential hyperbolic equation for the usual elastic displacement and the local spin precession equation (à la Landau–Lifshitz) of parabolic nature.

When thermal and dynamic effects are altogether discarded, Eqs. (21) and (26) reduce to the unique divergence equation

$$\frac{\partial}{\partial x_j} b_{ji} = 0, \quad (30)$$

with

$$b_{ji} = W \delta_{ji} - \sigma_{jk} u_{k,i} - H_{jk} w_{k,i}. \quad (31)$$

Such a formula was apparently proposed by Fan and Fan in 2008—also Fan ([2], pp. 301–302) under the name of generalized Eshelby energy–momentum tensor for the consideration of fracture in quasi-crystals with a generalization of the famous contour-independent J -integral of Rice given by the following configurational force:

$$F = \int_{\Gamma} \left(W n_1 - n_j \sigma_{ji} \frac{\partial u_i}{\partial x_1} - n_j H_{ji} \frac{\partial w_i}{\partial x_1} \right) d\Gamma. \quad (32)$$

This provides the driving force acting on the tip of a crack (encircled by a counterclockwise circuit Γ with ends on the free faces of a rectilinear crack extending possibly in the x_1 direction in the physical plane; \mathbf{n} = unit outward normal to Γ , n_1 = projection of \mathbf{n} in the x_1 direction). We note that Agiasofitou et al. [17] have also approached the matter of configurational forces in quasi-crystals in an original work dealing with defect properties.

4 Nonlinearity and plasticity of quasi-crystals

Nonlinearity usually calls for a formulation in finite strains and the introduction of geometrical nonlinearities together with physical nonlinearities. This is not the case here where we are satisfied with physical nonlinearities only. This primarily means a potential energy that is not quadratic in the relevant (small) deformation measures. Note that Eq. (3) is still formally valid in this case in the absence of thermodynamic irreversibilities. Should we know the mechanical response curves, we could in fact define the associated free energy by the formula proposed by Fan ([2], p. 295)

$$W(e_{ij}, w_{i,j}) = \int_0^{e_{ij}} \sigma_{ji} de_{ij} + \int_0^{w_{i,j}} H_{ji} dw_{ij}. \quad (33)$$

This does not tell much about the exact constitutive equations, save for the fact that the existence of a potential requires the absence of dissipation and the reversibility of the path in generalized stress–strain space.

However, for many engineers (see Chapter One in Ref. [18]) nonlinearity is synonymous with *plasticity*, i.e. an inherently dissipative behaviour marked by unloading along response curves that differ from those of the loading phases and thus exhibiting a kind of hysteresis (of course, in the absence of unloading, nobody can say that the body is not “simply” nonlinear elastic, even though of a special type!). The accompanying thermo-mechanical description of true plasticity is necessarily much more involved, and in spite of the presence and importance of structural defects in quasi-crystals, we do not know yet whether there is real need for a mathematical theory of plasticity of quasi-crystals expanded along the lines given in our book [19] for usual crystals. Such proposal is sketched out by Fan ([2], Sect. 14.2). This formulation proposing in parallel “plastic” evolution equations for both generalized strains e_{ij} and $w_{ij} \equiv w_{i,j}$, and including the effect of the phason stress H_{ij} on the generalized effective stress used to define the yield surface, may be surmised by analogy in the “Bak” inspired formulation, but it is doubtful in the “Lubensky” formulation where the phason displacement w_i itself already satisfies an evolution–diffusion equation.

5 Further comments and conclusion

In the foregoing sections, we have tried to elucidate some of the critical points concerning the continuum thermodynamics of quasi-crystals at the little cost of the implementation of now currently accepted formalisms. However, the main point remains that of the explicit writing of the coupled generalized “Hooke” constitutive equations when the relevant energy is simply jointly quadratic in the deformation measures (4), i.e. when Eq. (3) result in the linear relations

$$\sigma_{ji} = C_{jilk} e_{lk} + R_{jilk} w_{k,l}, \quad H_{ji} = K_{jilk} w_{k,l} + R_{lkji} e_{kl}, \quad (34)$$

wherein the only a priori admitted symmetries are

$$C_{jilk} = C_{(ji)(lk)} = C_{lkji}, K_{jilk} = K_{lkji}, R_{jilk} = R_{(ji)lk}. \quad (35)$$

Specific expressions of the tensor coefficients for various material symmetries admitting the existence of quasi-crystal symmetries are documented in Fan ([2]; Chapters 5, 6) and references therein. Fortunately, only a few nonzero coefficients are necessary in many of the applications for the so-called “one-dimensional” quasi-crystals (that are nonetheless three-dimensional structures, standard symmetry still applying in a plane orthogonal to this peculiar direction).

What remains unclear is the physical significance of a quantity such as the prescribed force of component g_i —when it exists—and of the “natural” boundary condition (involving the normal vector component $n_j H_{ji}$) for the phason field. The work of Cimmelli [19] does not help to answer this last query. But we should note that a possible interpretation was granted to the bulk force g_i by authors such as Ding et al. [20] who related it in some way to the first gradient of the phason eigen-distortion and phonon eigen-distortion, but this is outside continuum mechanics, per se. It can also be noted that there exists strong disagreement—accompanied by harsh comments—between tenants of various physical interpretations of dynamical properties of quasi-crystals (e.g. opposite schools represented by Coddens [21] and Francoual et al. [22] and further discussions by these authors). Finally, for the sake of completeness, we remark that a third path (midway between the “Bak” and “Lubensky” models) was recently proposed by Agiasofitou and Lazar [23] in which (2) is complemented by an elementary viscous term—equivalently, (8) is complemented by an inertial term—thus yielding a kind of telegraphy equation, while phonons remain giving rise to undamped elastic waves. This makes the model more classical and certainly less challenging than the original “Lubensky” model with its interpretation of an internal variable of state from the thermodynamic viewpoint.

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