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"Material" mechanics of materials

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Abstract

The paper outlines recent developments and prospects in the application of the continuum mechanics expressed intrinsically on the material manifold itself. This includes applications to materially inhomogeneous materials, physical effects which, in this vision, manifest themselves as quasi-inhomogeneities, and the notion of thermodynamical driving force of the dissipative progress of singular point sets on the material manifold with special emphasis on fracture, shock waves and phase-transition fronts.

1 General overview

"Material" mechanics, or "mechanics on the material manifold" or still, *Eshelbian mechanics* as we nicknamed it because of the original and essential contribution of J.D.Eshelby [1] inspired by field theory, is the mechanics of continua expressed on the material manifold so that, in contradistinction to the traditional formulation in physical space , it captures at once *true material inhomogeneities or quasi-inhomogeneities*. As shown exactly in recent years, the latter include field singularities of the line and surface types, thermal effects, and all gradient effects related to diffusive internal variables of state or to additional internal degrees of freedom. This obviously enhances the role of this mechanics in so far as the *thermomechanics* of materials - especially those endowed with a microstructure - is concerned. This contribution emphasizes this role and highlights the successes met during the last ten years.

2 True material inhomogeneities

The theory of material uniformity and inhomogeneity advocated by Epstein and Maugin in geometrical terms [2],[3] - following early works by W.Noll [4] and C.C.Wang [5] - yields a direct characterization of uniformity in terms of a *material* stress tensor $\mathbf{b}$ called the *Eshelby stress*. This is the energy dual of first-order *transplants* of the reference configuration in the same way as the first Piola-Kirchhoff stress $\mathbf{T}$ is the dual of the classical deformation gradient. Indeed, in *quasi-statics*, let $W(\mathbf{F};\mathbf{X})$ be the elastic energy per unit volume of a reference configuration K , where $\mathbf{F}$ is the deformation gradient with respect to K and $\mathbf{X}$ denotes the material coordinates. Then according to Epstein and the author, at each material point, we can remove the explicit dependence on $\mathbf{X}$, by effecting a local change $\mathbf{K}(\mathbf{X})$ of reference configuration so that, with $J_K = det\mathbf{K}$, we can write

$$W = \bar{W}\left(\mathbf{F};\mathbf{X}\right) = J_K^{-1}\tilde{W}\left(\mathbf{F}\mathbf{K}\left(\mathbf{X}\right)\right) = \hat{W}\left(\mathbf{F},\mathbf{K}\right) \tag{1}$$

and thus

$$\mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}\ ,\ \mathbf{b} = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}\ = -\frac{\partial \hat{W}}{\partial \mathbf{K}}\mathbf{K}^T\,. \tag{2}$$

It was further shown in *dynamical finite-strain elasticity* [6], [7] that the momentum associated with this stress flux is the so-called *pseudomomentum* P which plays a fundamental role in crystal physics (wave-momentum on a lattice) and in electromagnetic optics. The corresponding volume source term $\mathbf{f}^{inh}$, if any, is the " material " force of *inhomogeneity* which displays at once the possible *explicit* (i .e., *not* through the fields) dependence of material properties (whether mechanical or else) on the material point, i.e., material inhomogeneity *per se*. More precisely, we have the local *balance of pseudomomentum* at $\mathbf{X}$ in the form

$$\frac{\partial P}{\partial t} - div_R\mathbf{b} = \mathbf{f}^{inh}, \tag{3}$$

wherein

$$P \equiv \frac{\partial L}{\partial \mathbf{V}},\ \mathbf{b} = -\ \left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right)\ ,\ \mathbf{f}^{inh}\colon = \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{\exp l}\ , \tag{4}$$

with

$$L = K - W\left(\mathbf{F};\mathbf{X}\right)\ ,\ K = \frac{1}{2}\rho_0\left(\mathbf{X}\right)\mathbf{V}.\mathbf{C}.\mathbf{V},\ \ \mathbf{C} \equiv \mathbf{F}^T.\mathbf{F}\ , \tag{5}$$

Here $\mathbf{V}$ is the material velocity based on the " inverse motion " $\mathbf{X} = \chi^{-1}\left(\mathbf{x},t\right)$, i.e.,

$$\mathbf{V}\ =\ \left.\frac{\partial\chi^{-1}}{\partial t}\right|_x\ .$$

Remark 1 *It must be emphasized that the above mentioned material force of inhomogeneity posseses no energetic contents and it does not cause dissipation (compare below). In that sense, such forces may be called fictitious.*

3 Quasi-inhomogeneity forces

All fields such as temperature q in a heat conductor or internal variables of state α (reflecting some irreversibility) which have not reached a spatially uniform state, are shown to produce source terms in the balance of the above-mentioned pseudomomentum [8],[9].They are manifestations of so-called *quasi-inhomogeneities* which play in many respects the same role as true material inhomogeneties (this should not be overlooked in *fracture applications*). For instance, in *materially homogeneous* elastic conductors of heat, eqn.(3) is replaced by

$$\frac{\partial P}{\partial t} - div_R\mathbf{b} = \mathbf{f}^{th},\ \mathbf{f}^{\mathrm{th}}\colon = S\nabla_R\theta\,, \tag{6}$$

where S is the entropy per unit volume in K and the W present in the definition of L in eqn.$(4)_2$ is necessarily the *free energy* per unit volume. As clearly shown by the first of eqns.(6), a nonzero gradient of temperature gives rise to a material force just like a true material inhomogeneity. In the case of a dissipative internal variable α with dual thermodynamical force $A = -(\partial W/\partial\alpha)$, we have in addition in the right-hand side of eqn.$(6)_1$ a material force given by [9]

$$\mathbf{f}^{\alpha} := A\,\nabla_R\alpha\,, \tag{7}$$

while the corresponding *dissipated power* reads :

$$\Phi^{\alpha} = A.\dot{\alpha} \;= A.\left.\frac{\partial\,\alpha}{\partial\,t}\right|_x - \mathbf{f}^{\alpha}.\mathbf{V}, \tag{8}$$

where a superimposed dot indicates the material time derivative and the time derivative at x fixed is the Eulerian time derivative.

The above scheme applies to weakly nonlocal damage or elastoplasticity.

Remark 2 *The presence of true or quasi-inhomogeneities can be interpreted in geometrical terms as rendering the material manifold a non-Riemannan one (this is the case with continuously distributed dislocations and also of thermoelasticity and magnetoelasticity which are quasi-plastic phenomena). -see, e.g., Chapter 6 in ref.[10].*

Remark 3 *The multiplicative decomposition* **FK** *present in eqn.(1) is tantamount to saying that the stress tensor* **b** *is the driving force governing a local structural rearrangement. This is the case in elastoplasticity or in certain phase transitions. As a matter of fact the material mapping* **K** *may be interpreted as the inverse of the plastic deformation "gradient" in plasticity theories based on a multiplicative decomposition of* **F**. *In that case* **FK** *is none other than the elastic deformation "gradient". Such theories, where the Eshelby stress tensor in the so-called intermediate or elastically-released configuration plays the rôle of driving force, have been developed accordingly [11], [12], [13], [14]. More precisely, the Mandel stress usually given by* $\mathbf{M} = \mathbf{S}.\mathbf{C}$, *where* **S** *is the second Piola-Kirchhoff (fully material) stress known in such theories in fact is the non-isotropic part of the Eshelby material stress tensor. It is then natural that this tensor plays also a fundamental role as the relevant stress in the notion of reduced-shear stress in studying criteria of activation of dislocations [15]. The present considerations find another application in the theory of material growth such as developed by Epstein and Maugin [26] with applications by Imatani and*

Maugin [27]. As a matter of fact, the above-given developments allow one to show that the three most creative lines of thoughts in the continuum mechanics of materials in the second half of the 20th century - the finite deformation line with its multiplicative decomposition, the geometrical line with the works of Kondo, Bilby, Kröner, Noll and Wang, and the configurational-force line with Eshelby and others, are strongly interrelated and find a grand unification with the two dual notions of local material rearrangement and Eshelby material stress tensor (for this aspect, see Maugin [28]).

4 Driving forces on singularity sets

Thermodynamic forces driving field singularities in thermoelasticity (or more complex constitutive descriptions) have been shown to belong to the above-highlighted class of material forces. The singularity sets of interest (and the only ones in three-dimensional space) are points, lines and walls [16] (transitions zones of physically non zero thickness but viewed mathematically as singular surfaces of zero thickness). In the case of *brittle fracture* (line of singularity viewed as a point, the crack tip, in a planar problem) and the progress of *discontinuity fronts* (phase-transition fronts and shock waves) which are singular surfaces of the first order in Hadamard's classical classification) one shows exactly that *dissipation* is strictly related to the power expanded by such forces in the irreversible progress of the singularity set.

For instance, in brittle fracture (where fracture occurs in the elastic regime), we have the following two essential results of what we call the *analytical theory of brittle fracture*. The *material force* **F** acting on the tip of a straight through crack and the corresponding *energy-release rate* G are given by the equations [17]:

$$F = -\lim_{\delta \to 0} \int_{\Gamma(\delta)} \{L\mathbf{N} - P\left(\bar{\mathbf{V}}.\mathbf{N}\right)\} dA \tag{9}$$

and

$$G = \lim_{\delta \to 0} \int_{\Gamma(\delta)} H\left(\bar{\mathbf{V}}.\mathbf{N}\right) dA \ , \tag{10}$$

respectively, with the following exact result as δ goes to zero:

$$G = \bar{\mathbf{V}}.F \geq 0 \ . \tag{11}$$

Here $H = K + W$, is the Hamiltonian density per unit reference volume, $\bar{\mathbf{V}}$ is the material velocity of the crack tip, $\Gamma(\delta)$ is a sequence of notches of end radius δ converging uniformly to the crack and the crack tip as δ goes to zero, and the inequality sign in the second part of eqn.(11) reflects the second law of thermodynamics since expression $(11)_1$ is the power dissipated in the domain change due to the irreversible progress of the crack inside the body.

Extensions of these results were made to the case of *coupled fields* useful in developing smart materials and structures, including the cases of nonlinear electroelasticity [18], magnetoelasticities of paramagnets [19] and ferromagnets [20], and polar crystals [21]. The formulation in fact is *canonical* and applies to many cases with the appropriate replacement of symbols by physical fields. In the case of elastoplasticity with hardening a J-integral can be constructed using this formalism [11]. Furthermore, the very form taken by eqn.(3) in cases more complex than pure elasticity, e.g.., the source term $(6)_2$ or (7), provides a hint at generalization of formula (9) in the case of inhomogeneous, dissipative, thermo-deformable conductors; viz. (3) is replaced at any regular material point $\mathbf{X}$ by

$$\frac{\partial P}{\partial t} - div_R \mathbf{b} = \mathbf{f}^{inh} + \mathbf{f}^{th} + \sum\nolimits_{\alpha} \mathbf{f}^{\alpha}. \tag{12}$$

It is readily shown that (9) then transforms to the general formula:

$$\begin{aligned} F = & \int_\Gamma \left\{ \mathbf{N}.\mathbf{b} + P\left(\bar{\mathbf{V}}.\mathbf{N}\right)\right\} dA - \tfrac{d}{dt}\int_G P\, dV + \\ & \int_G \left(\mathbf{f}^{inh} + \mathbf{f}^{th} + \sum\nolimits_\alpha \mathbf{f}^\alpha\right) dV, \end{aligned} \tag{13}$$

where Γ is a circuit (in the counter clockwise direction) enclosing the domain G around the crack tip, starting from the lower face of the (traction free) crack and ending on its upper face. This gives a means to study analytically or numerically the influence of full dynamics, material inhomogeneities (e.g., inclusions), thermal effects, and, e.g., elastoplasticity or damage (represented by the set of α variables) in the vicinity of the crack tip.

In the case of discontinuity fronts in thermoelastic solids, basing on the inclusive notion of *Massieu function*, the *Hugoniot* and *Gibbs functionals* appear to be the relevant material driving forces ; the classical theories of shock waves and nondissipative phase-transition fronts (obeying Maxwell's rule) appear then to be extreme singular cases of the theory [22],[23]. This was dealt with in great detail in recent papers. It suffices to remind the reader that in the absence of dislocations at the front - so-called *coherent* front - the phase-transition front progress is shown to be strictly normal and the driving force, called *Hugoniot-Gibbs* force H_{PT} , is none other than the jump of the double normal component of the " quasi-static " part (no kinetic energy contribution) of the Eshelby stress tensor expressed on the basis of the *free* energy W (the front is homothermal) , i.e., symbolically,

$$H_{PT} = \mathbf{N}.\left[\mathbf{b}_S\left(W\right)\right].\mathbf{N}. \tag{14}$$

The dissipation per unit surface at the front Σ is given by (compare to (11))

$$\Phi_\Sigma = -H_{PT}\,\bar{V}_N \geq 0\ , \tag{15}$$

where $\bar{V}_N$ is the normal velocity of the front. This corresponds to the presence of a generally nonvanishing localized *hot heat source* at Σ . Whenever we impose that H_{PT} vanishes identically although there is effective progress of the front, we are in the situation of the *nondissipative* Landau's theory of phase transitions, and the vanishing of H_{PT} corresponds exactly to the *Maxwell rule of equal areas* (or construction of the *Maxwell line* ; no hysteresis in the physical response). This is a *singular* and somewhat irrealistic case in phase-transition theory where dissipation and hysteresis in the physical response are generally observed.

Another such *singular* case is found in the study of the propagation of *shock waves* where, in the absence of a true shock structure, the celebrated *Hugoniot relation* is given by the identical vanishing of the driving force H_S where this *Hugoniot functional* (i.e., depending on the state on both sides of the front) is given by

$$H_S = \mathbf{N}.\left[\mathbf{b}_S\left(E\right)\right].\mathbf{N}\,, \tag{16}$$

where $\mathbf{b}_S\,(E)$ is the quasi-static part of the Eshelby stress based on the *internal* energy. The vanishing condition H_S =0 shows the artificiality of the " classical " shock-wave theory since, to be consistent with the condition of entropy growth at the front, there should indeed be dissipation at the front which propagates dissipatively. This dissipation, logically, should be related to the power dissipated by the driving force in the motion of the front. Unfortunately this driving force was classically set equal to zero in spite of a possible progress. The general theory [21], [22] resolves this paradox by re-establishing a proper thermodynamical frame in accord with Eshelbian mechanics. For instance, it is shown for a general front (shock-wave of phase-transition front) that a single thermodynamic Massieu potential, or *generating function* M can be introduced, at the front, such that the following two exact relations hold true :

$$\sigma_\Sigma = [M] \geq 0 \ , \ \mathbf{f}_\Sigma.\bar{\mathbf{V}} = [\theta\, M] \ , \tag{17}$$

where σ_Σ is the rate of entropy growth at Σ, and $\mathbf{f}_\Sigma$ is the co-vectorial dissipative driving force acting on Σ. Clearly, for a homothermal phase-transition front eqns.(17) yield the result expressed by eqn.(15) with $H_{PT} = -\,\mathbf{f}_\Sigma.\mathbf{N}$. Otherwise, as it should, the entropy growth at a shock wave involves both the power expanded by the driving force and the jump of temperature since then

$$\sigma_\Sigma = \langle\theta\rangle^{-1}\left\{\mathbf{f}_\Sigma.\bar{\mathbf{V}} - \langle M\rangle\,[\theta]\right\} \geq 0. \tag{18}$$

Generalizations of this formulation to electrodeformable and magnetodeformable media, and to media already presenting a bulk intrinsic dissipation (e.g., of the viscous or plastic type represented by the a set of internal variables) are more or less straightforward.

5 Other applications

Other applications devised include the driving of the non-inertial motion of *solitonic structures* viewed as localized defects on the material manifold - or *quasi-particles* -, a presently developing theory of material growth in the bulk or by accretion (further work in progress by M.Epstein, S.Imatani, S.Quiligotti and the author), and the conception of numerical methods or algorithms based on Eshelbian mechanics, e.g. the minimization of parasite driving forces on the material manifold due to a bad design of finite-difference schemes (C.I.Christov and the author [24], [25]) or finite-element discretization (M.Braun, P.Steinmann and the author), and the design of a cellular automaton using the notion of thermodynamical driving force (A.Berezovski and the author). In all cases, the Eshelby stress is the driving force responsible for local material rearrangements and the balance of pseudomomentum in local PDE or jump form, or in integrated form, plays the fundamental role in both theory and applications, with a special emphasis of the latter in *micromechanics*.

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"Materijalna" mehanika materijala

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Rad sadrži nedavni razvoj i perspektive u primeni mehanike kontinuuma izražene pomoću materijalne mnogostrukosti same po sebi. Ovo uključuje primene materijalno nehomogenih materijala, fizičke efekte koji se, ovakvim načinom gledanja, manifestuju kao kvazi-nehomogenosti kao i pojam termodinamički pokretačke sile disipativnog razvoja skupova singularnih tačaka na materijalnoj mnogostrukosti sa specijalnom primenom na lom, udarne talase i frontove faznih transformacija.