



The non-local generalized standard approach: a consistent gradient theory

Quoc-Son Nguyen^{a,*}, Stéphane Andrieux^b

^a Laboratoire de mécanique des solides, CNRS (umr7649), École polytechnique, Palaiseau, France

^b Laboratoire de mécanique des structures industrielles durables, EDF-CNRS (umr2832), Clamart, France

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Abstract

In this Note, the generalized standard approach is proposed as a consistent gradient theory to include the gradients of the temperature and of the internal parameter in the set of state variables. This theory is derived from a global point of view, developing the basic ideas of continuum thermodynamics. It leads to the appropriate expressions of the entropy and of the internal energy in terms of the free energy in the case of temperature gradient. The local governing equations of the proposed thermodynamical approach are derived. The formalism of the dissipation potential can be applied in the same spirit as in the classical description from the dissipation analysis. **To cite this article:** *Q.-S. Nguyen, S. Andrieux, C. R. Mecanique 333 (2005)*. © 2004 Académie des sciences. Published by Elsevier SAS. All rights reserved.

Résumé

Le modèle standard généralisé non local : une théorie consistante du gradient. On propose dans cette Note une théorie du gradient basée sur une formulation du modèle standard généralisé pour inclure d'une manière simple et consistante les gradients de la température et des paramètres internes comme des variables d'état supplémentaires. Cette théorie est construite à partir d'une formulation globale des idées de base de la thermodynamique des milieux continus. On montre que la présence du gradient de température conduit à des expressions appropriées de l'entropie et de l'énergie interne en fonction de l'énergie libre. Les équations locales du modèle thermodynamique proposé sont ensuite données. Le formalisme du potentiel de dissipation s'applique comme dans le cadre de la théorie classique à partir de l'analyse de la dissipation. **Pour citer cet article :** *Q.-S. Nguyen, S. Andrieux, C. R. Mecanique 333 (2005)*.

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* Corresponding author.

E-mail addresses: son@lms.polytechnique.fr (Q.-S. Nguyen), stephane.andrieux@edf.fr (S. Andrieux).

Version française abrégée

On propose dans cette Note une description thermodynamique incluant les gradients de température et de paramètre interne comme variables d'état additionnelles. Cette description constitue une version non locale du modèle des matériaux standard généralisés [10], adaptée à la présence des gradients dans l'expression de l'énergie. Un bref survol de la littérature permet de rappeler les résultats existant sur les théories du gradient. D'une manière générale, presque tous les modèles discutés depuis plus de deux décennies suggèrent une modification soit du bilan du premier principe, soit de l'expression du second principe par des termes additionnels d'origine mécanique ou thermique, cf. par exemple cf. [1,4,6,7,2,8,5,9]. Ce sont essentiellement des discussions développant les approches de Frémond cf. [1], et de Maugin [2], proposées initialement pour le traitement des paramètres internes. Le modèle développé ici consiste à adapter l'approche standard généralisée à la prise en compte des gradients de température et de paramètre interne. La présence de ces gradients dans les variables d'état conduit à raisonner d'une manière globale, en termes de champs pour un solide avant de manipuler les grandeurs locales. Ainsi, l'énergie libre d'un solide de volume V est une fonctionnelle dépendant des champs de température, de déplacement et de paramètre interne. La force généralisée d'entropie est, au signe près, la dérivée de l'énergie libre globale par rapport au champ de température et représentée par une forme linéaire (8). Dans le même esprit, l'expression globale de l'énergie interne permet de définir la densité d'énergie interne en fonction de la densité d'énergie libre (11). Le cadre thermodynamique proposé est enfin décrit d'une façon globale ou locale par les énoncés des deux principes avec les expressions appropriées de la production d'entropie et de l'énergie interne. Il conduit à des expressions associées des dissipations intrinsèque et thermique (18), (20). Dans le même esprit, le paramètre interne contribue à la dissipation intrinsèque d'un solide par une forme linéaire du champ de vitesse de paramètre interne. Son expression s'obtient simplement et permet de nouveau d'appliquer le formalisme des matériaux standard généralisés pour l'écriture des lois complémentaires (26). En particulier, ces résultats permettent de mieux comprendre la signification physique des lois complémentaires, qui s'écrivent sous la forme des équations locales de volume et des conditions aux limites naturelles comme par exemple dans les Éqs. (27). En particulier, les équations locales pour un solide Ω sont données par (26) dans le cas d'un potentiel de dissipation locale de la forme $D(\dot{\alpha}, \nabla \dot{\alpha})$.

1. Introduction

In the last two decades, many discussions have been devoted to the problem of strain localization, especially in the numerical computation of elastic-plastic softening or damaged weakening solids. A possibility to avoid thin localization or mesh-dependence problems is to introduce the gradient of the plastic strain or the damage parameter fields in order to penalize possible sharp localizations. The introduction of the gradient of these internal parameters can be done in different ways, at the level of the plastic or damage yield values as well as at the expression of the driving forces, cf. [1–3] and to the quoted references therein. In particular, the method proposed in [1] and in [4] gives an original approach generalizing the classical second gradient theory of elasticity by an additional virtual work equation. A different and interesting method consists of adding entropy fluxes or sources in the entropy production, cf. [2,5]. These methods have been applied in various applications such as in plasticity and in damage mechanics [6,7,5]. They have been also adopted to include the thermal gradient, cf. [8,9].

A consistent gradient theory is presented here, in order to contribute to the discussions of the literature. The proposed approach is a non-local version of the generalized standard model [10] and appears as a direct extension of the classical formalism of continuum thermodynamics associated with the introduction of gradients.

2. The non-local generalized standard approach

2.1. The classical framework of continuum thermodynamics

In classical thermodynamics and in a Lagrangian description, it is well known that the free energy w per unit volume of a solid is related to the internal energy e and the entropy s per unit volume by

$$e = Ts + w(T, \nabla u, \alpha), \quad s = -w_{,T} \quad (1)$$

where T denotes the temperature, u the displacement and α a set of internal parameter, $(T, \nabla u, \alpha)$ is a system of state variable of the material. For any material volume V , the first and second principles when taking account of the dynamical equation, can be written as

$$\begin{cases} \dot{E} = P_i + P_{\text{cal}} \\ P_{\text{entr}} = \dot{S} + \int_V \frac{q}{T} \cdot n \, da \geq 0 \\ E = \int_V e \, dV, \quad P_i = \int_V B : \nabla \dot{u} \, dV, \quad P_{\text{cal}} = - \int_{\partial V} q \cdot n \, da, \quad S = \int_V s \, dV \end{cases} \quad (2)$$

where E is the internal energy of V , P_i the internal mechanical work, P_{cal} the heat supply, S the entropy of V , B is the unsymmetric Lagrangian stress. These equations also lead to the local equations

$$\begin{cases} \dot{e} + \nabla \cdot q = B : \nabla \dot{u} \\ p_{\text{entr}} = \dot{s} + \nabla \cdot \frac{q}{T} \geq 0 \end{cases} \quad (3)$$

If the free energy depends also on the temperature and internal parameter gradients i.e. if

$$w = w(T, \nabla T, \nabla u, \alpha, \nabla \alpha) \quad (4)$$

it is already known from the existing discussions in the literature that some of Eqs. (1), (3) cannot remain available.

2.2. The global point of view

For any material volume V , the associated free energy

$$\mathbf{W}(\mathbf{T}) = \int_V w(T, \nabla T, \nabla u, \alpha, \nabla \alpha) \, dV \quad (5)$$

is a functional of the fields \mathbf{T} , \mathbf{u} , α and admits as derivative with respect to \mathbf{T} the linear form $\mathbf{W}_{,\mathbf{T}}[\delta\mathbf{T}]$ defined by

$$\mathbf{W}_{,\mathbf{T}}[\delta\mathbf{T}] = \int_V (w_{,T} \delta T + w_{,\nabla T} \cdot \nabla \delta T) \, dV \quad (6)$$

The global point of view consists of relating a global thermodynamical force to the global energy as its functional derivative, for example $\mathbf{S} = -\mathbf{W}_{,\mathbf{T}}$ since from (1), this relationship also holds in classical thermodynamics.

2.3. The entropy

The definition of the associated entropy force in the global sense

$$\mathbf{S} = -\mathbf{W}_{,\mathbf{T}} \quad (7)$$

means that

$$\begin{cases} \mathbf{S}[\delta\mathbf{T}] = \int_V (\eta \delta T + \eta' \cdot \nabla \delta T) \, dV \\ \text{with } \eta = -w_{,T}, \quad \eta' = -w_{,\nabla T} \end{cases} \quad (8)$$

In this expression, η and η' represent respectively the local force parameters associated with T and ∇T . The classical notion of a scalar entropy is replaced here by the pair (η, η') .

2.4. The internal energy

The internal energy of the solid, which can be again related to the free energy of the solid by the generalized Legendre transform despite the lack of symmetry of the pair (\mathbf{s}, \mathbf{T})

$$\mathbf{E} = \mathbf{S}[\mathbf{T}] + \mathbf{W}(\mathbf{T}) \quad (9)$$

where \mathbf{S} and \mathbf{T} are associated by (8), is also an additive function with respect to V when \mathbf{T} is continuous. If $-\mathbf{W}(\mathbf{T})$ is a convex function, then $\mathbf{E}(\mathbf{s})$ is a convex function. This statement follows from the fact that $\mathbf{E}(\mathbf{S})$ then satisfies

$$\mathbf{E}(\mathbf{S}) = \max_{\mathbf{T}} \mathbf{S}[\mathbf{T}] + \mathbf{W}(\mathbf{T}) \quad (10)$$

and is a convex function as a upper-envelope of linear functions. It is interesting to underline that the convexity of $-\mathbf{W}(\mathbf{T})$ is ensured if the function $-w(T, \nabla T, \nabla u, \alpha, \nabla \alpha)$ is convex with respect to the variables $(T, \nabla T)$.

The local expression of the internal energy can be easily derived in terms of w . Indeed, since from (9)

$$\mathbf{E} = \int_V (-w_{,T} T - w_{,\nabla T} \cdot \nabla T + w) dV = \int_V e dV$$

it is concluded that the following local equation holds

$$e = -w_{,T} T - w_{,\nabla T} \cdot \nabla T + w \quad (11)$$

As expected, the internal energy e is obtained from the energy $-w$ by the local Legendre transform with respect to the two independent variables $(T, \nabla T)$, of dual variables (η, η') :

$$\begin{cases} e(\eta, \eta', \nabla u, \alpha, \nabla \alpha) = \eta T + \eta' \cdot \nabla T + w(T, \nabla T, \nabla u, \alpha, \nabla \alpha) \\ \eta = -w_{,T}, \quad \eta' = -w_{,\nabla T}, \quad T = e_{,\eta}, \quad \nabla T = e_{,\eta'} \end{cases} \quad (12)$$

Under the assumption of convexity of $-w(T, \nabla T, \nabla u, \alpha, \nabla \alpha)$ with respect to the variables $(T, \nabla T)$, the convexity of $e(\eta, \eta', \nabla u, \alpha, \nabla \alpha)$ with respect to the variables (η, η') is ensured.

2.5. The proposed framework

A particular and interesting model consists of extending the classical formalism of thermodynamics with some new and global definitions. The following energy balance is thus assumed:

$$\begin{cases} \dot{\mathbf{E}} = P_i + P_{\text{cal}} + P_c \\ \mathbf{E} = \mathbf{S}[\mathbf{T}] + \mathbf{W} \end{cases} \quad (13)$$

for the first principle where P_c denotes an extra energy supply due to the neighbouring interaction following Frémond's ideas (cf. [1,4,11,8] for this and for the connecting discussions)

$$P_c = \int_{\partial V} n \cdot (b \cdot \dot{\alpha} + c \cdot \dot{T}) da \quad (14)$$

b and c denote two internal generalized forces generated by the energy exchange inside a volume and associated respectively with $\dot{\alpha}$ and \dot{T} in the similar way as the stress tensor B which is associated with \dot{u} . For a given solid Ω , the value of $b \cdot n$ and $c \cdot n$ on its boundary must be zero when there is no extra energy supply from the external world, for example on a free boundary or a surface separating the solid with a classical medium. For a volume $V \subset \Omega$, the expression of these forces in terms of the state variables will be subsequently discussed.

The second principle is written as

$$\begin{cases} P_{\text{entri}} = P_{\text{entr}} - P_{\text{entre}} \\ P_{\text{entr}} = \int_V p_{\text{entr}} dV, \quad p_{\text{entr}} = \frac{1}{T} (T \dot{\eta} + \nabla T \cdot \dot{\eta}') = \frac{1}{T} \dot{e}_{(\nabla u, \alpha)} \\ P_{\text{entre}} = - \int_{\partial V} p_{\text{entre}} da, \quad p_{\text{entre}} = \frac{q}{T} \cdot n \end{cases} \quad (15)$$

where the production entropy p_{entr} per unit reference volume is identified from the variation $\dot{e}_{(\nabla u, \alpha)}$ of the internal energy at the present values of non-thermal variables, i.e. $(\nabla u, \alpha, \nabla \alpha)$ are maintained fixed. If ∇T disappears in the expression of the free energy, then the classical description is recovered with $\eta = s$.

Since these equations are available for all V , finally the proposed framework is also governed by the following local equations

$$\begin{cases} \dot{e} + \nabla \cdot q = B : \nabla \dot{u} + \nabla \cdot (b \cdot \dot{\alpha} + c \cdot \dot{T}) \\ e = \eta T + \eta' \cdot \nabla T + w, \quad \eta = -w, T, \quad \eta' = -w, \nabla T \\ p_{\text{entri}} = \dot{\eta} + \frac{\nabla T}{T} \cdot \dot{\eta}' + \nabla \cdot \frac{q}{T} \geq 0 \end{cases} \quad (16)$$

where $P_{\text{entri}} = \int_V p_{\text{entri}} dV$ and p_{entri} denotes the internal entropy production per unit reference volume.

2.6. The thermal and intrinsic dissipations

The following definition of the intrinsic dissipation of the solid is now introduced:

$$D_{\text{int}} = \dot{\mathbf{S}}[\mathbf{T}] - P_{\text{cal}} \quad (17)$$

with the Helmholtz condition that the system of state variables $(T, \nabla T, \nabla u, \alpha, \nabla \alpha)$ must be a normal system. This means that the intrinsic dissipation D_{int} must be zero when the non-thermal variables are maintained fixed for all $(\dot{T}, \nabla \dot{T})$ and for all V . Since $D_{\text{int}} = \int_V d_{\text{int}} dV$ with

$$d_{\text{int}} = T \dot{\eta} + \nabla T \cdot \dot{\eta}' + \nabla \cdot q \quad (18)$$

thus

$$\begin{cases} p_{\text{entri}} = \frac{d}{T}, \quad d = d_{\text{int}} + d_{\text{ther}} \geq 0 \\ d_{\text{ther}} = -q \cdot \frac{\nabla T}{T} \end{cases} \quad (19)$$

By definition, d_{int} is the intrinsic dissipation and d_{ther} the thermal dissipation per unit reference volume. From the local equation of energy (16), the definition (18) leads to

$$d_{\text{int}} = T \dot{\eta} + \nabla T \cdot \dot{\eta}' + \nabla \cdot q = (B - w, \nabla u) : \nabla \dot{u} - w, \alpha \cdot \dot{\alpha} - w, \nabla \alpha \cdot \nabla \dot{\alpha} + \nabla \cdot (b \cdot \dot{\alpha} + c \cdot \dot{T}) \quad (20)$$

It follows that

$$\int_{\partial V} \dot{T} c \cdot n da = 0 \quad \forall \dot{T}, \forall V \quad \text{thus } c = 0 \quad (21)$$

It is well known that the Fourier law $q = -k \nabla T$ ensures $d_{\text{ther}} \geq 0$ and leads from (20) to the following thermal equation:

$$T \dot{\eta} + \nabla T \cdot \dot{\eta}' - k \Delta T = (B - w, \nabla u) : \nabla \dot{u} - w, \alpha \cdot \dot{\alpha} - w, \nabla \alpha \cdot \nabla \dot{\alpha} + \nabla \cdot (b \cdot \dot{\alpha}) \quad (22)$$

2.7. The dissipation potential

From (20) and (21), the intrinsic dissipation of a solid V is:

$$D_{\text{int}} = \int_V B^{IR} : \nabla \dot{u} dV + \int_V (-w, \alpha \cdot \dot{\alpha} - w, \nabla \alpha \cdot \nabla \dot{\alpha} + \nabla \cdot (b \cdot \dot{\alpha})) dV$$

In this expression, the first term is the dissipation due to the irreversible stress $B^{IR} = B - B^R$, $B^R = w, \nabla u$. The remaining term, which is the dissipation due to the internal parameters, can also be written as the linear form $\mathbf{A}[\dot{\alpha}]$

$$\mathbf{A}[\dot{\alpha}] = \int_V (\nabla \cdot w, \nabla \alpha - w, \alpha) \cdot \dot{\alpha} dV + \int_{\partial V} n \cdot (b - w, \nabla \alpha) \cdot \dot{\alpha} da \quad (23)$$

Again, the formalism of dissipation potential may be applied. For the sake of clarity, let us assume that the displacement is not an irreversible mechanism, thus $B^{IR} = 0$ and the intrinsic dissipation is reduced to $\mathbf{A}[\dot{\alpha}]$.

2.7.1. Dissipative couplings

If a dissipation potential $\mathbf{D}^V(\dot{\alpha})$ exists for a solid V then the following complementary laws hold:

$$\mathbf{A} = \mathbf{D}^V(\dot{\alpha}),_{\dot{\alpha}} \quad (24)$$

The particular case of a dissipation potential of the form

$$\mathbf{D}^V(\dot{\alpha}) = \int_V D(\dot{\alpha}, \nabla \dot{\alpha}) dV \quad (25)$$

can be introduced in order to discuss the case of volume dissipative mechanisms. From (24) the following local complementary relationships hold:

$$\begin{cases} \nabla \cdot w_{,\nabla\alpha} - w_{,\alpha} = D_{,\dot{\alpha}} - \nabla \cdot D_{,\nabla\dot{\alpha}} & \forall x \in V \\ (b - w_{,\nabla\alpha}) \cdot n = D_{,\nabla\dot{\alpha}} \cdot n & \forall x \in \partial V \end{cases} \quad (26)$$

A system of partial differential equations with a set of appropriate natural boundary conditions are thus obtained. In particular, for a given solid Ω submitted to a classical thermal and mechanical loading, the complementary relationships give the system of partial differential equations with boundary conditions

$$\begin{cases} \nabla \cdot w_{,\nabla\alpha} - w_{,\alpha} = D_{,\dot{\alpha}} - \nabla \cdot D_{,\nabla\dot{\alpha}} & \forall x \in \Omega \\ (w_{,\nabla\alpha} + D_{,\nabla\dot{\alpha}}) \cdot n = (b \cdot n)^d = 0 & \forall x \in \partial\Omega \end{cases} \quad (27)$$

The system of Eqs. (27) has been considered in various discussions, cf. [12,5,13].

2.7.2. Reversible couplings

In this case, there is no dissipation and the following governing equations are obtained

$$\begin{cases} \nabla \cdot w_{,\nabla\alpha} - w_{,\alpha} = 0 & \forall x \in \Omega \\ w_{,\nabla\alpha} \cdot n = 0 & \forall x \in \partial\Omega \end{cases} \quad (28)$$

Note that if \mathbf{W} is convex with respect to the field α , then

$$\alpha = \mathbf{Arg} \min_{\beta} \mathbf{W}(\mathbf{T}, u, \beta)$$

2.7.3. Thermodynamic restrictions

For a volume V , the global intrinsic dissipation D_{int} is non-negative if the potential $\mathbf{D}^V(\dot{\alpha})$ is a convex functional and takes its minimum value for $\dot{\alpha} = 0$. In order to ensure a positive intrinsic dissipation per unit volume, the intrinsic dissipation must be positive for all volume V . Thus Eqs. (26) must be satisfied for all V . Since the vector n can be then chosen arbitrarily, it follows that

$$b = w_{,\nabla\alpha} + D_{,\nabla\dot{\alpha}} \quad (29)$$

From (26) and from this expression of b in terms of the energy w and of the dissipation potential D , it is checked that

$$d_{\text{int}} = -w_{,\nabla\alpha} \cdot \nabla \dot{\alpha} - w_{,\alpha} \cdot \dot{\alpha} + \nabla \cdot (b \cdot \dot{\alpha}) = D_{,\dot{\alpha}} \cdot \dot{\alpha} + D_{,\nabla\dot{\alpha}} \cdot \nabla \dot{\alpha} \quad (30)$$

Thus d_{int} is non-negative if the local potential $D(\dot{\alpha}, \nabla \dot{\alpha})$ is a convex function with respect to the pair of independent variables $(\dot{\alpha}, \nabla \dot{\alpha})$, and takes its minimum value at $(0, 0)$ since the right-hand side of (30) is then non-negative.

In this case, the system of complementary local laws and appropriate boundary conditions (27) for a given solid Ω can also be obtained in a global way from the minimum principle

$$\dot{\alpha} = \mathbf{Arg} \min_a \int_{\Omega} (D(a, \nabla a) + w_{,\alpha} \cdot a + w_{,\nabla\alpha} \cdot \nabla a) d\Omega. \quad (31)$$

2.8. Remarks

– It is interesting to compare the obtained results concerning the thermal gradient to Cardonna et al. discussion [8]. They privileged the classical relation $e = Ts + w$ while our approach preserves the duality (11). The final expressions concerning the intrinsic and thermal dissipations are the same in both approaches.

– Our approach also works to include higher order gradients of temperature. For example, if the free energy is $w = w(T, \nabla T, \nabla \nabla T, \nabla u, \alpha, \nabla \alpha)$, then the same method leads to

$$\begin{cases} e = \eta T + \eta' \cdot \nabla T + \eta'' \cdot \nabla \nabla T + w \\ \eta = -w_{,T}, \quad \eta' = -w_{,\nabla T}, \quad \eta'' = -w_{,\nabla \nabla T} \\ \mathbf{S}[\delta \mathbf{T}] = \int_V (\eta \delta T + \eta' \cdot \nabla \delta T + \eta'' \cdot \nabla \nabla \delta T) dV \\ p_{\text{entr}} = \frac{1}{T} (T \dot{\eta} + \nabla T \cdot \dot{\eta}' + \nabla^2 T \cdot \dot{\eta}'') \end{cases} \quad (32)$$

3. Conclusion

The proposed non-local generalized standard model is a new approach to include the gradients. It gives a natural and consistent gradient theory. The model results from the basic ideas of continuum thermodynamics with some proper assumptions in order to take into account the presence of the temperature gradient. It gives some new suggestions on the subject and contribute to the existing discussions in the literature. In particular, it proposes an appropriate and original expression of the internal energy and of the entropy production.

For the modeling of the internal parameter gradient, the expression of the intrinsic dissipation as a linear form of the rate of the internal parameter field in a solid gives the possibility to apply the formalism of the dissipation potential. It offers also a firm thermodynamical basis for some existing gradient theories of damage and of plasticity, which can be recast into the general formalism proposed here but for which the question of thermodynamical admissibility has not been addressed yet (see [13] or [3] for some examples).

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