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MECHANICS

Thermodynamic consistency of third grade finite strain elasticity

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Abstract. The thermodynamic framework of finite strain viscoelasticity with second order weak nonlocality in the deformation gradient is investigated. The application of Liu's procedure leads to a class of third grade elastic materials where the second gradient of the stress appears in the elastic constitutive relation. Finally the dispersion relation of longitudinal plane waves is calculated in isotropic materials.

Key words: continuum mechanics, higher grade elasticity, weakly nonlocal nonequilibrium thermodynamics, Liu's procedure, double wave equation.

1. INTRODUCTION

Thermodynamic requirements are important in all theoretical approaches of continuum mechanics. The classical form of the Clausius–Duhem inequality [1] does not allow higher than first grade elasticity [2] and plasticity [3] without any further ado. Therefore, new concepts such as higher order stresses and configurational forces emerged to circumvent this condition and to understand the thermodynamic compatibility of successful material models [4–6].

In this paper we show that a weakly nonlocal extension of the constitutive state space does not contradict the Second Law and leads to constitutive relations of higher grade finite strain elasticity and viscoelasticity that are compatible with rigorous thermodynamic methods and requirements. Our method is based on two basic observations, which are different from the classical framework of Gurtin [2], namely that

– the entropy flux is a constitutive quantity,
– for higher order weakly nonlocal state spaces the gradient of the balances and other kinematic constraints result in further constraints on the entropy inequality.

The assumption of a *constitutive entropy flux* is a straightforward generalization of the Gibbs–Duhem inequality, and one can prove that in simple cases it leads to the classical form and to the classical results both in irreversible thermodynamics [7] and in thermoelasticity in particular [8]. This generalization is well accepted and applied beyond mechanics [9–11]. With the assumption of a constitutive entropy flux Liu's and Coleman–Noll procedures are equivalent (see [12] for a proof in a particular case).

It is also remarkable that further constraints in Liu's procedure result in more general constitutive functions [13]. Our main result, the thermodynamic admissibility of the dependence of constitutive functions on space derivatives of the deformation gradient, is the consequence of this general property of the entropy

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inequality. Therefore we do not need to introduce higher order stresses (or any other additional physical concepts) in advance, but at the end we will see that some of the consequences of our method can be interpreted in those terms. The introduction of the gradient of local constraints (e.g. balances) in nonequilibrium thermodynamics is a mathematical necessity in the case of higher order weakly nonlocal constitutive state spaces – overlooked by Gurtin in [2] – and has a unifying power to understand the role of the Second Law in several seemingly different theories of continuum physics (see e.g. [14] and the references therein).

In this paper we apply our method with Liu's procedure in third grade elasticity ([1], p. 63), where the constitutive state space depends on the second space derivative of the deformation gradient. Therefore third grade elasticity is classified as a second order weakly nonlocal theory. We prove the thermodynamic admissibility of a class of constitutive relations with two remarkable properties:

– the second order derivatives of the deformation appear without explicitly introducing double stress in advance as an independent theoretical concept,
– the second derivative of the stress is part of the nondissipative stress–strain constitutive relation. This is similar to the suggestion of Aifantis (see [15] and the references therein).

We also derive a simple dispersion relation of longitudinal plane waves to demonstrate the properties of the constitutive relation.

2. CONTINUUM IN A PIOLA–KIRCHHOFF FRAMEWORK

All quantities are defined on the reference configuration. The substantial time derivative is denoted by a dot and the material space derivative is ∂_i, where $i \in \{1,2,3\}$. Higher order derivatives are denoted by more indices, e.g. ∂_{ij} is the second gradient, χ^i is the motion, $F^i_j = \partial_j \chi^i$ is the deformation gradient.

According to the traditional concept of objectivity [16], this kinematic standpoint ensures the objectivity of the whole treatment as long as the constitutive quantities depend on objective physical quantities. However, the original mathematical formulation of the concept of objectivity by Noll is questionable [17,18], and a generalization based on precise spacetime notions and a four-dimensional formalism was suggested to improve it [19,20]. In this work we do not apply this generalized objective framework, our results are derived by usual three-dimensional notions. However, we exploit some consequences of this generalization to simplify our calculation. First of all it will be convenient to work in a Piola–Kirchhoff framework, where the balances and the physical quantities are interpreted in the reference configuration (see [5,21] for a similar treatment). The first Piola–Kirchhoff stress will be denoted as a tensor. As we have mentioned above, a constitutive state space spanned by Noll-objective physical quantities (e.g., right Cauchy–Green deformation) could ensure the objectivity of the whole treatment. However, it is more convenient to work with the deformation gradient, the material velocity, and the total energy as basic variables. Moreover, this choice of state variables is not forbidden by our generalized notion of objectivity. We will partially change to Noll-objective quantities at the end introducing the internal energy with the usual definition and show a particular stress–strain relation with a Cauchy deformation measure.

Therefore in our treatment of the constitutive theory of third grade elastic materials the constitutive state space is based on the following fields: $v^i, \partial_j v^i, \partial_{jk} v^i, F^i_j, \partial_k F^i_j, \partial_{kl} F^i_j, e, \partial_i e$. Here v^i is the velocity, F^i_j is the deformation gradient, and e is the specific total energy. Our approach is second order weakly nonlocal in the velocity and the deformation gradient, and first order weakly nonlocal in the energy. It is usual to avoid introducing a velocity field as an independent variable by working with internal energy and internal energy balance. However, as the velocity and deformation gradient fields form a single physical quantity, we find instructive to show that the direct definition of internal energy can be introduced at the end and that the total energy filtered through Liu's procedure can give the same results when specified to local constitutive relations. This is the approach that we have followed in the case of relativistic fluids, where the Liu procedure was essential to distinguish total and internal energies [22].

The well-known kinematic relation between the velocity and the deformation gradient

$$\dot{F}^i_j - \partial_j v^i = 0 \tag{1}$$

is introduced as a constraint for the entropy inequality together with the balances.

The balance of linear momentum is

$$\rho_0 \dot{v}^i - \partial_j T^{ij} = 0^i. \tag{2}$$

Here ρ_0 is the material density and T^{ij} is the first Piola–Kirchhoff stress, introduced as a tensor. The balance of total energy is

$$\rho_0 \dot{e} + \partial_i q^i = 0, \tag{3}$$

where q^i is the energy flux. As we are working in a second order weakly nonlocal constitutive state space the derivative of the kinematic relation (1) and the momentum balance (2) are additional constraints according to the exploitation method of weakly nonlocal continuum theories [23,24]:

$$\begin{aligned} \partial_k \dot{F}^i_j - \partial_{kj} v^i &= 0^i_{jk}, && (4) \\ \rho_0 \partial_j \dot{v}^i + \partial_{jk} T^{ik} &= 0^i{}_j. && (5) \end{aligned}$$

The gradient of the energy balance does not give an additional constraint, because the constitutive state space is first order weakly nonlocal in the energy.

The entropy inequality requires that

$$\rho_0 \dot{s} + \partial_i J^i \geq 0,$$

where s is the specific entropy and J^i is the material entropy flux. Here we are looking for restrictions on the constitutive functions T^{ij}, q^i, J^i in terms of the entropy density derivatives. It is important to see that the derivative of the momentum balance extends the process direction space, which is spanned by the first and also the second space derivatives of the constitutive state space.

We introduce $\Lambda^j_i, \lambda_i, \kappa, \Lambda^{jk}_i, \lambda^j_i$ Lagrange–Farkas multipliers of equations (1)–(5), respectively. Therefore the starting point of the Liu procedure is the following inequality:

$$\begin{aligned} 0 \leq & \rho_0 \dot{s} + \partial_i J^i - \Lambda^j_i (\dot{F}^i_j - \partial_j v^i) - \lambda_i (\rho_0 \dot{v}^i - \partial_j T^{ij}) - \kappa(\rho_0 \dot{e} + \partial_i q^i) \\ & - \Lambda^{jk}_i (\partial_k \dot{F}^i_j - \partial_{kj} v^i) - \lambda^j_i (\rho_0 \partial_j \dot{v}^i + \partial_{kj} T^{ik}) \\ = & \rho_0 \frac{\partial s}{\partial v^i} \dot{v}^i + \rho_0 \frac{\partial s}{\partial \partial_j v^i} \partial_j \dot{v}^i + \rho_0 \frac{\partial s}{\partial \partial_{jk} v^i} \partial_{jk} \dot{v}^i + \rho_0 \frac{\partial s}{\partial F^i_j} \dot{F}^i_j + \rho_0 \frac{\partial s}{\partial \partial_k F^i_j} \partial_k \dot{F}^i_j \\ & + \rho_0 \frac{\partial s}{\partial \partial_{kl} F^i_j} \partial_{kl} \dot{F}^i_j + \rho_0 \frac{\partial s}{\partial e} \dot{e} + \rho_0 \frac{\partial s}{\partial \partial_i e} \partial_i \dot{e} \\ & + \frac{\partial J^j}{\partial v^i} \partial_j v^i + \frac{\partial J^k}{\partial \partial_j v^i} \partial_{kj} v^i + \frac{\partial J^l}{\partial \partial_{kj} v^i} \partial_{lkj} v^i + \frac{\partial J^k}{\partial F^i_j} \partial_k F^i_j + \frac{\partial J^l}{\partial \partial_k F^i_j} \partial_{lk} F^i_j \\ & + \frac{\partial J^m}{\partial \partial_{lk} F^i_j} \partial_{mlk} F^i_j + \frac{\partial J^i}{\partial e} \partial_i e + \frac{\partial J^j}{\partial \partial_i e} \partial_{ji} e \\ & - \kappa \left(\rho_0 \dot{e} + \frac{\partial q^j}{\partial v^i} \partial_j v^i + \frac{\partial q^k}{\partial \partial_j v^i} \partial_{kj} v^i + \frac{\partial q^l}{\partial \partial_{kj} v^i} \partial_{lkj} v^i + \frac{\partial q^k}{\partial F^i_j} \partial_k F^i_j + \frac{\partial q^l}{\partial \partial_k F^i_j} \partial_{lk} F^i_j \right. \\ & \left. + \frac{\partial q^m}{\partial \partial_{lk} F^i_j} \partial_{mlk} F^i_j + \frac{\partial q^i}{\partial e} \partial_i e + \frac{\partial q^j}{\partial \partial_i e} \partial_{ji} e \right) \end{aligned}$$

$$
\begin{aligned}
&-\lambda_r\left(\rho_0\dot{v}^r-\frac{\partial T^{rj}}{\partial v^i}\partial_j v^i-\frac{\partial T^{rk}}{\partial\partial_j v^i}\partial_{kj}v^i-\frac{\partial T^{rl}}{\partial\partial_{kj}v^i}\partial_{lkj}v^i-\frac{\partial T^{rk}}{\partial F^i_j}\partial_k F^i_{\ j}-\frac{\partial T^{rl}}{\partial\partial_k F^i_j}\partial_{lk}F^i_{\ j}\right.\\
&\left.-\frac{\partial T^{rm}}{\partial\partial_{lk}F^i_j}\partial_{mlk}F^i_{\ j}-\frac{\partial T^{ri}}{\partial e}\partial_i e-\frac{\partial T^{rj}}{\partial\partial_i e}\partial_{ji}e\right)-\Lambda_i^j(\dot{F}^i_{\ j}-\partial_j v^i)\\
&-\lambda_r^s\left(\rho_0\partial_s\dot{v}^r-\frac{\partial T^{rj}}{\partial v^i}\partial_{sj}v^i-\partial_j v^i\partial_s\left[\frac{\partial T^{rj}}{\partial v^i}\right]-\frac{\partial T^{rk}}{\partial\partial_j v^i}\partial_{skj}v^i-\partial_{kj}v^i\partial_s\left[\frac{\partial T^{rk}}{\partial\partial_j v^i}\right]\right.\\
&-\frac{\partial T^{rl}}{\partial\partial_{kj}v^i}\partial_{slkj}v^i-\partial_{lkj}v^i\partial_s\left[\frac{\partial T^{rl}}{\partial\partial_{kj}v^i}\right]-\frac{\partial T^{rk}}{\partial F^i_j}\partial_{sk}F^i_{\ j}-\partial_k F^i_{\ j}\partial_s\left[\frac{\partial T^{rk}}{\partial F^i_j}\right]\\
&-\frac{\partial T^{rl}}{\partial\partial_k F^i_j}\partial_{slk}F^i_{\ j}-\partial_{lk}F^i_{\ j}\partial_s\left[\frac{\partial T^{rl}}{\partial\partial_k F^i_j}\right]-\frac{\partial T^{rm}}{\partial\partial_{lk}F^i_j}\partial_{smlk}F^i_{\ j}-\partial_{mlk}F^i_{\ j}\partial_s\left[\frac{\partial T^{rm}}{\partial\partial_{lk}F^i_j}\right]\\
&\left.-\frac{\partial T^{ri}}{\partial e}\partial_{si}e-\partial_i e\,\partial_s\left[\frac{\partial T^{ri}}{\partial e}\right]-\frac{\partial T^{rj}}{\partial\partial_i e}\partial_{sji}e-\partial_{ji}e\,\partial_s\left[\frac{\partial T^{rj}}{\partial\partial_i e}\right]\right)\\
&-\Lambda_i^{jk}(\partial_k\dot{F}^i_{\ j}-\partial_{kj}v^i).
\end{aligned}
$$

The time derivative related Liu equations imply that Lagrange–Farkas multipliers are determined by the entropy derivatives, and that the specific entropy and the stress do not depend on the highest derivatives of the constitutive state space $s=s(v^i,\partial_j v^i,F^i_{\ j},\partial_k F^i_{\ j},e)$.

Then, the Liu equations related to the highest order space derivatives determine the entropy flux in the following form

$$
J^i=\frac{\partial s}{\partial e}q^i-\frac{\partial s}{\partial\partial_i v^r}\left(\frac{\partial T^{jr}}{\partial e}\partial_j e+\frac{\partial T^{kr}}{\partial\partial_l v^m}\partial_{lk}v^m+\frac{\partial T^{kr}}{\partial\partial_l F^n_m}\partial_{lk}F^n_{\ m}\right)+K^i.
$$

Here $K^i=K^i(v^i,\partial_j v^i,F^i_{\ j},\partial_k F^i_{\ j},e)$ is the extra entropy flux with the above denoted restricted functional dependences. Then we introduce several convenient assumptions in order to get a simple and solvable form of the dissipation inequality. First of all we define the classical heat flux $\hat{q}$ and also the internal energy of the third grade viscoelastic material including an isotropic kinetic energy contribution of deformation gradient rate:

$$
u:=e-\frac{1}{2}v^i v_i-\frac{\alpha_1}{2}(\dot{F}^i_i)^2-\frac{\alpha_2}{2}\dot{F}^i_{\ j}\dot{F}^j_{\ i},\qquad \hat{q}^i:=q^i+v_jT^{ij}.
$$

Moreover, we may observe that a particular choice of the extra entropy flux reduces the dissipation inequality to a solvable form. Therefore we assume that

$$
K^i:=\frac{\partial s}{\partial e}v_jT^{ij}-\frac{\partial s}{\partial\partial_i F^k_j}\partial_j v^k.
$$

Finally the temperature θ is defined by the entropy derivatives $\frac{\partial s}{\partial e}=\frac{\partial s}{\partial u}=\frac{1}{\theta}$ and the free energy as $\psi(\mathbf{F},\nabla\mathbf{F}):=u-\theta s$. Then we obtain

$$
\theta\sigma_S=\theta\hat{q}^i\partial_i\frac{1}{\theta}+\partial_j v^i\left(T_i^j-\frac{\partial\psi}{\partial F^i_j}-\alpha_1\partial_{lk}T^{lk}\delta_i^j-\alpha_2\partial^j_{\ k}T^k_{\ i}+\partial_k\frac{\partial\psi}{\partial\partial_k F^i_j}\right)\geq 0. \qquad (6)
$$

The first two terms in the parentheses of the above expression are the classical terms from second grade elasticity. The very last term in (6) resembles the double stress relation that one can get by virtual power techniques.

In the nondissipative case, assuming constant material parameters, we get a constitutive relation of third grade elasticity in the following form

$$\mathbf{T} - \nabla \cdot (\alpha_1 (\nabla \cdot \mathbf{T})\mathbf{I} + \alpha_2 \nabla \mathbf{T}) = \frac{\partial \psi}{\partial \mathbf{F}} - \nabla \cdot \frac{\partial \psi}{\partial \nabla \mathbf{F}}. \tag{7}$$

3. SIMPLE WAVES

We may calculate the dispersion relation of a one-dimensional plane wave in the small strain approximation in order to check some consequences of the above stress–strain relation.

Let us assume a usual isotropic quadratic free energy for symmetric strains $\varepsilon^i_j = \frac{1}{2}(F^i_{\ j} + F^{\ j}_i - 2\delta^i_j)$, that is second order isotropic quadratic also in the gradient of the symmetric strains. Then, according to representation theorems, only two additional material parameters a_1, a_2 appear in the free energy function [25]

$$\psi(\varepsilon^i_j, \partial_k \varepsilon^i_j) = \frac{\lambda}{2}(\varepsilon^i_i)^2 + \mu \varepsilon^i_j \varepsilon^i_j + \frac{a_1}{2}\partial_i \varepsilon^j_j \partial^i \varepsilon^k_k + \frac{a_2}{2}\partial_i \varepsilon^j_k \partial^i \varepsilon^k_j.$$

Then we get

$$T^{\ j}_i - \alpha_1 \partial_k \partial_l T^{lk} \delta^j_i - \alpha_2 \partial_k \partial^j T^{\ k}_i = \lambda \varepsilon^k_k \delta^j_i + 2\mu \varepsilon^j_i - a_1(\partial^k_k \varepsilon^l_l)\delta^j_i - a_2 \partial^k_k(\varepsilon^j_i).$$

Let us investigate the simplest one-dimensional case and reduce the treatment to one component of the above tensorial equation. Introducing the notation $T = T^{11}$ and $\varepsilon = \varepsilon^{11}$ and also denoting ∂_1 by a dash we get

$$T - \alpha T'' = \hat{\lambda}\varepsilon - a\varepsilon'',$$

where $\alpha = \alpha_1 + \alpha_2$, $\hat{\lambda} = \lambda + 2\mu$, and $a = a_1 + a_2$. This constitutive relation is coupled to the balance of momentum that is in our case

$$\rho_0 \ddot{\varepsilon} - T'' = 0.$$

Assuming constant material parameters, we get the following dispersion relation

$$\omega^2 = \frac{k^2(\hat{\lambda} + ak^2)}{\rho_0(1 + \alpha k^2)}.$$

The characteristic feature of this dispersion relation is that the small wavelength and large wavelength limits result in finite acoustic phase velocities:

$$\lim_{k\to 0} \frac{\omega(k)}{k} = \sqrt{\hat{\lambda}/\rho_0}$$

and

$$\lim_{k\to\infty} \frac{\omega(k)}{k} = \sqrt{a/(\alpha\rho_0)}$$

as demonstrated in Fig. 1. This kind of behaviour is a property of the double wave equation [26]. Double wave equations are introduced by microstructural considerations, e.g. in microstrain theories or internal variable theories [25,27].

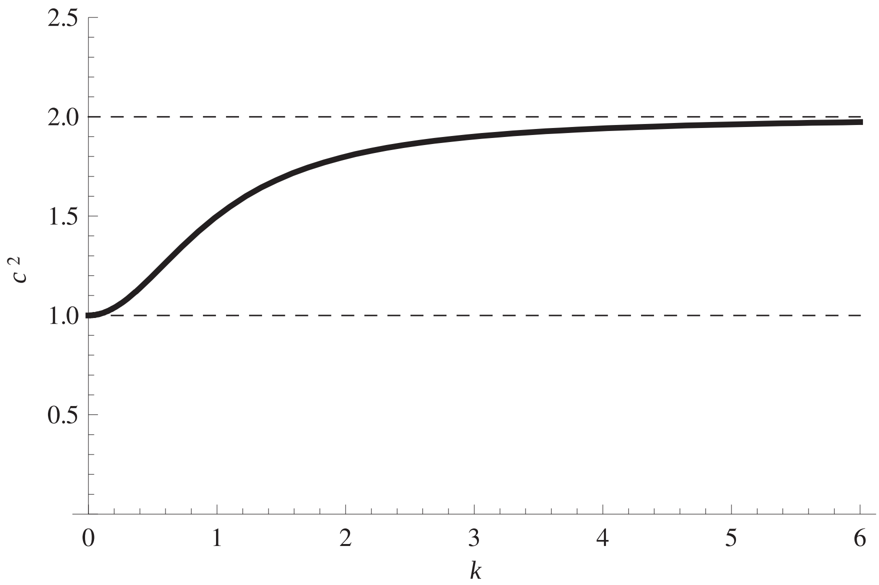

Fig. 1. The square of the phase velocity $v^2 = (\omega(k)/k)^2$ with the parameter values $\rho_0 = 1$, $\hat{\lambda} = 1$, $\alpha = 1$, and $a = 2$.

4. SUMMARY

In this paper we investigated a weakly nonlocal extension of viscoelasticity up to second order in the deformation gradient. The entropy flux was considered as a constitutive quantity and we applied the Liu procedure introducing also the gradients of the balance of momentum and of the kinematic relation (1) as constraints on the entropy balance.

The calculations were performed in the Piola–Kirchhoff framework. The constitutive state space was chosen according to the generalization of the Noll principle of frame indifference introducing the components of the velocity–deformation gradient mixed four-tensor and their first and second space derivatives as constitutive variables.

A complete solution of Liu's equations was calculated and a particular form of the entropy flux and the dissipation inequality were obtained. In order to solve the dissipation inequality, we introduced some simplifications. In particular, a quadratic form of the kinetic energy and some further related rearrangements resulted in a form where Onsagerian fluxes and forces can be identified. The constitutive relation of the nondissipative mechanical material contains the gradients of the pressure in addition to the classical terms and the usual form of the constitutive relation of the double stress appeared without postulating such term in advance.

It is important to note that the extension of the constitutive state space toward higher order gradients does not change the obtained form of (6) as long as only the first derivatives of (1) and (2) are introduced as additional constraints. This extension results in simple explicit solutions of the nondissipative differential stress–deformation relation and then (7) can be considered as a constitutive relation of third grade elasticity.

We calculated also a one-dimensional dispersion relation and concluded that it was similar to the dispersion relation of some microstructured materials as one could expect in the case of higher grade solids (see e.g. [28]).

As we mentioned in the Introduction, stress–strain relations similar to (7) were already proposed in the literature [15]. However, there the motivation was to remove stress singularities with a kind of ad hoc "reaction diffusion" form. Here we showed that this kind of extension is compatible with a weakly nonlocal thermodynamic framework, there are natural boundary conditions coming from the requirement of vanishing entropy flux, and a physical origin of stress derivative terms is the modified (isotropic) kinetic energy related to the rate of the deformation gradient.

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Kolmandat järku lõpliku deformatsiooni elastsuse termodünaamiline käsitlus

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On uuritud teist järku nõrga mittelokaalsusega lõplike deformatsioonidega viskoelastsusteooria termodünaamilist raamistikku. Liu meetodi rakendamine viib teist järku elastsete materjalide klassini, mille elastne olekuvõrrand sisaldab teist pingegradienti. On välja arvutatud tasandpikilainete dispersiooniseos.