

THERMODYNAMICALLY CONSISTENT GRADIENT ELASTICITY WITH AN INTERNAL VARIABLE

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ABSTRACT. The role of thermodynamics in continuum mechanics and the derivation of proper constitutive relations is a topic discussed in Rational Mechanics. The classical literature did not use the accumulated knowledge of thermostatics and was very critical of the heuristic methods of irreversible thermodynamics. In this paper, a small strain gradient elasticity theory is constructed with memory effects and dissipation. The method is nonequilibrium thermodynamics with internal variables; therefore, the constitutive relations are compatible with thermodynamics by construction. The thermostatic Gibbs relation is introduced for elastic bodies with a single tensorial internal variable. The thermodynamic potentials are first-order weakly nonlocal, and the entropy production is calculated. The constitutive functions and the evolution equation of the internal variable are then constructed. The second law analysis has shown a contribution of gradient terms to the stress, also without dissipation.

1. Introduction

Rational mechanics was developed with a sharp criticism of the mathematics used in continuum mechanics [67, 68]. However, the criticism went far beyond some suggested methodological improvements. A complete reorganisation of fundamental aspects was proposed from two main points of view: the representation of spacetime and the representation of thermodynamic principles. In the following, we survey these aspects and argue that methods of nonequilibrium thermodynamics are under the principles of continuum mechanics in general and with elasticity in particular. In [75] small strain linear elasticity was analysed, and the most important aspects were summarised. In the following, after the discussion of objectivity and thermodynamic aspects, we extend these previous results and obtain a dissipative gradient theory of small strain elasticity with a weakly nonlocal internal variable.

2010 *Mathematics Subject Classification:* 74A15; 74A60.

Key words and phrases: nonequilibrium thermodynamics, generalised continua, gradient elasticity.

2. Objectivity

Objectivity is the concept of spacetime representation of physical quantities and laws. Spacetime representation is particularly important in nonrelativistic continuum mechanics and closely related to the principle of material frame indifference [22], a concept whose mathematical formulation was developed by Noll. This formulation requires transformation rules between reference frames [54]. Later on, Noll's deeper analysis led to a mathematical structure based on affine spaces, but without a detailed spacetime model [55–57]. In a complete spacetime formulation, the physical quantities, their governing differential equations as well as the constitutive functions can be given in an absolute form, that is, without any reference frames and independently of the flow of the material [43]. In this framework, a physical theory is reference frame independent by construction. However, a complete formulation meets conceptual difficulties, including the simplest possible case of one-component simple fluids. One of the key difficulties is to establish a frame independent concept of energy, because kinetic energy, including the density of kinetic energy of a one-component simple fluid, $K = \frac{\rho v^2}{2}$, cannot be frame independent, being defined by the relative velocity. Therefore, it is zero when the reference frame is fixed to the fluid and not zero in any other reference frame. An absolute formulation requires the use of four quantities, spacetime vectors and tensors, also in a nonrelativistic framework, where the time is absolute, and space is relative. Therefore, a spatial, three-dimensional space vector or tensor cannot be frame independent, whereas a four-dimensional spacetime vector or tensor can. This observation appears indirectly in the transformation rule based definition by Noll, too [44]. In a complete spacetime formulation, transformation rules are not parts of the definition of objectivity and can be avoided completely [73]. Then the frame independence of the Gibbs relation and the entropy production can be proved. This formulation is compatible with the related concepts of Rational Extended Thermodynamics [52, 63, 79] and also with special relativity [78]. The consequences of spacetime formulation for kinematics lead to a generalisation that does not require the existence of a stress-free, relaxed state of any continua in a finite deformation theory [26].

It is remarkable that the formalism of four quantities is not always necessary and can be safely avoided. It is also important to understand how far we can go with the help of our customary three-dimensional vectors and tensors. The following aspects of nonrelativistic spacetime are to be considered:

- The four vector representation of physical quantities makes it inevitable that the density of an extensive physical quantity, ρ_{ext} and its current density, \mathbf{j}_{ext} , are parts of the same absolute four quantity. This is also apparent in a nonrelativistic, more properly Galilean relativistic framework. For example, conductive and convective current densities, \mathbf{j}_{cond} and $\rho_{ext}\mathbf{v}$, are related with the formula $\mathbf{j}_{tot} = \mathbf{j}_{cond} + \rho_{ext}\mathbf{v}$. This is the transformation rule between comoving and laboratory frames of the spatial part of a four vector, where the timelike component is the density, and the spacelike component is the current density in a particular reference frame.

- Spacetime derivatives are four covectors. Spacelike components of four covectors are absolute, but timelike components transform, and they differ depending on reference frames. For example, the relation of a local, partial time derivative in a laboratory frame, ∂_t , to a substantial time derivative, $\frac{d}{dt}$, of the form $\frac{d}{dt} = \partial_t + \mathbf{v} \cdot \nabla$ is a transformation rule of the timelike component of the spacetime derivative between a laboratory reference frame and a reference frame comoving with the fluid. Then, the gradients are spacelike covectors and do not transform at all. This fact is well hidden using Noll's definition.

A consequence of these observations is that gradient dependent constitutive functions are frame independent, but one should be careful with time derivatives. It is also easy to comprehend that a balance is a four divergence and, therefore, frame independent.

In the following, the application of these simple rules ensures that we obtain frame independent theories with the usual tools of three-dimensional tensor analysis. The simple but not customary four-dimensional affine spaces of nonrelativistic spacetime are not necessary; one can focus on the main subject of the paper – the formulation of thermodynamic principles.

3. Second law of thermodynamics

Rational mechanics considers the second law as a foundation of constitutive modelling in continuum mechanics. However, concepts from thermostatics, like the Gibbs relation with differentials, were abandoned, and the convenient and simple methods of classical irreversible thermodynamics with thermodynamic fluxes and forces are mostly rejected as mathematically inexact [66]. The criticism was well deserved since obscure concepts cannot lead far, and the development of irreversible thermodynamics slowed down. Despite many efforts, classical irreversible thermodynamics was unable to enter into the realm of continuum mechanics. The studies of the most critical challenges, time and space nonlocalities, that is, rheology and gradient theories, do not use irreversible thermodynamics, except some notable but not influential results [11, 36–38, 85]. The breakthrough of the last fifty years, Extended Thermodynamics, was the result of ideas from kinetic theory and much less the consequence of a rigorous rational methodology [34, 40]. The rigorous approach encountered the inadequate formulation of objectivity, chose kinetic theory as a basis and established the concept of objectivity rejecting the definition by Noll [50, 52, 53].

On the other hand, the rigorous mathematical approach did not result in the expected general and universal theory extending the modelling power of continuum theories but effectively blocked some research directions, in particular toward weakly nonlocal extensions. In their influential paper, Coleman and Gurtin proved that weakly nonlocal internal variables are incompatible with the second law [13] and, in another paper, Gurtin argued that gradient elasticity is incompatible with the second law [27]. Therefore, theories of spatial interactions were developed in a different direction, mostly without the direct constructive application of

thermodynamic principles [1, 2, 7, 9, 15, 20, 21, 48, 59, 83] or with the help of brand new concepts, like phase fields [60, 61], interstitial working, extra fluxes [18, 19] or microforce balance [28, 29, 31]. In these theories, the importance of the second law varies, but, in general, does not play a constructive role. The big idea of the principle-based rational approach has encountered difficulties with the complicated memory functional material models and faced mathematical problems, because the constitutive theory leads to unavoidable and physically unacceptable instabilities in gradient elasticity [17, 33, 51].

However, one may realise that the problem with rational methodology is not the use of mathematics, but the rigid attitude of finding the correct physical starting points. The conditions of a theorem are to be scrutinised from a physical point of view and modified if necessary. For example, the rigorous methods of second law analysis, the Coleman-Noll and Liu procedures [14, 42], can be extended to obtain weakly nonlocal constitutive functions with three conditions:

- The entropy flux is a constitutive quantity, and it is not always equal to the heat flux divided by temperature.
- The spatial derivative of a constraint can be considered as an additional constraint, depending on the structure of the constitutive state space.
- Thermodynamics fluxes and forces are available concepts for solving the entropy inequality.

The first condition, the idea of treating the entropy flux as a constitutive quantity originated from the work by Müller [49] and was later refined by Verhás and Nyíri [58, 84]. It is also a spacetime question, since entropy density and entropy flux are parts of the same objective physical quantity, the entropy four vector. Then one can show that classical irreversible thermodynamics is a first-order weakly nonlocal constitutive theory with balances as constraints and the thermodynamic flux-force system appears naturally [69]. The extended Coleman–Noll and Liu procedures are applicable for checking the second law compatibility of weakly nonlocal continuum theories [12, 70] and can be applied for constructing new ones or unifying independent looking theoretical developments, like internal variables with generalised continua or phase field evolution [5, 72, 74, 76, 81].

Also, the Gibbs relation of thermostatics is a source of information that should be understood; otherwise, we neglect the related accumulated experience from physics and chemistry. The critical aspect here is the extension of the concept of extensivity in situations where its original definition is seemingly not applicable, for example to elasticity and gradient effects. These are the topics of the next sections.

4. Thermostatics of elasticity

In the following, we use index notation in a small strain theory, where the strain is denoted by ε^{ij} . Here the indices are spatial and upper-lower index pairs denote summation, e.g. ε_i^i is the trace of the strain tensor. The indices are abstract, that is, they do not denote any coordinates, only the tensorial properties of the spatial physical quantities in the three-dimensional vector space of the position.

The distinction of upper-lower indices is not always essential, because the three-dimensional relative space is endowed with the Euclidean metric, and one may therefore identify vectors with covectors. This kind of abstract index notation was introduced by Penrose in relativity theories [62], and its use and advantage in nonrelativistic (i.e. Galilean relativistic) spacetime were explained in [73].

Deformation or strain cannot be extensive thermodynamic state variables in the classical sense. They are locally defined quantities, but homogeneous deformation of a finite volume continuum body depends on the shape of the body. Therefore, thermodynamic potentials of the complete body do not reflect material properties. In some thermodynamic books the Gibbs relation for elasticity appears as an analogon of the fluid Gibbs relation, but specific volume is substituted by strain [39, 47, 85]. Other handbooks about continuum mechanics do not consider homogeneous bodies at all [47], even when considering thermodynamic requirements [4, 30, 65]. However, strain is a local concept by definition and it is not necessary to start from quantities of the whole body in a continuum thermodynamic approach. The basic question here is the separation of the local strain from local rotation and the local Riemannian metric, which is responsible for the energy changes in the body [26]. Starting from local expressions, one can build up extensivity from this direction [6]. In the following we will introduce only small strains, where these problems can be solved relatively easily. Then the specific entropy, s , of elastic bodies is the function of the internal energy, e , and the strain, ε^{ij} , a second order symmetric tensor. Its partial derivatives are:

$$(4.1) \quad s = s(\mathbf{e}, \varepsilon^{ij}), \quad \frac{\partial s}{\partial \mathbf{e}} = \frac{1}{T}, \quad \frac{\partial s}{\partial \varepsilon^{ij}} = -\mathbf{v} \frac{\sigma_{ij}}{T},$$

where σ_{ij} is the thermostatic stress, \mathbf{v} is the specific volume and T is the temperature. Therefore, the Gibbs relation is written as

$$(4.2) \quad d\mathbf{e} = T ds + \mathbf{v} \sigma_{ij} d\varepsilon^{ij}.$$

The first order Euler homogeneity is ensured by introducing the chemical potential, μ , as

$$(4.3) \quad \mu := \mathbf{e} - T s - \mathbf{v} \sigma_{ij} \varepsilon^{ij}.$$

Then it is easy to obtain the particular expressions with densities as well:

$$(4.4) \quad d\rho_e = T d\rho_s + \sigma_{ij} d\varepsilon^{ij} + \left(\mu + \frac{\sigma_{ij} \varepsilon^{ij}}{\rho} \right) d\rho, \\ \rho_e = T \rho_s + \sigma_{ij} \varepsilon^{ij} + \mu \rho,$$

where $\rho = 1/\mathbf{v}$ is the density, $\rho_e = \rho e$ is the internal energy density, and $\rho_s = \rho s$ is the entropy density. It is easy to prove these expressions according to (4.2) and (4.3). Density changes are also not negligible in case of small strains. The quantities for the entire elastic body are calculated by multiplying the strain with the mass of the body M and then $M \varepsilon^{ij}$ will be the bulk, body-related extensive thermodynamic state variable if it is interpretable. Chemical potential is rarely introduced explicitly in continuum mechanics because mass exchange usually does not play a role. One can convert the previous expressions with the help of free energy density, f , defined

by the following Legendre transformation: $f = \rho_e - T\rho_s = \sigma_{ij}\varepsilon^{ij} + \mu\rho$, and then the Gibbs relation for densities (4.4) can be written as

$$(4.5) \quad df = -\rho_s dT + \sigma_{ij} d\varepsilon^{ij} + \frac{f}{\rho} d\rho, \quad \rightarrow \quad \rho d\frac{f}{\rho} = -\rho_s dT + \sigma_{ij} d\varepsilon^{ij}.$$

Seemingly there is no need for chemical potential at all. It is substituted by the specific free energy on the left-hand side of the previous expression. One can avoid the use of entropy and chemical potential starting from free energy in thermodynamical considerations of continuum mechanics [6, 10, 30], where one should take care of the variables of the previous functions. For example, free energy density has the natural variables: temperature, T , strain ε^{ij} and density ρ , as is apparent from the first Gibbs relation of (4.5). With the classical thermodynamical, differential-based representation of the Gibbs relation one can keep the flexibility of classical thermodynamics when changing the variables. One can see that with specific quantities the number of variables is reduced; while the free energy density is a function of three variables, $f(T, \varepsilon^{ij}, \rho)$, the specific free energy is the function of two, only, $\frac{f}{\rho}(T, \varepsilon^{ij})$. This is the consequence of extensivity, the first-order Euler homogeneity of the entropy of homogeneous bodies, here considered directly for locally defined specific quantities and densities [6].

For ideal elastic bodies, elastic energy is to be subtracted from the internal energy. Then, one may have two basic choices. In the following, the specific quantities are preferred, and specific elastic energy is therefore to be subtracted from the specific internal energy, and the specific entropy is given in the following form

$$s(e, \varepsilon^{ij}) = s\left(e - \mu\varepsilon^{ij}\varepsilon_{ij} - \frac{\lambda}{2}(\varepsilon^i_i)^2\right),$$

where the Lamé coefficients are $\hat{\mu} = \rho\mu$ and $\hat{\lambda} = \rho\lambda$, because $\rho_{ela} = \hat{\mu}\varepsilon^{ij}\varepsilon_{ij} + \frac{\hat{\lambda}}{2}(\varepsilon^i_i)^2$ is the density of the elastic energy. Using the definition of temperature as the derivative of the entropy in (4.1), and assuming constant μ, λ parameters, one obtains, that

$$(4.6) \quad \sigma^{ij} = 2\hat{\mu}\varepsilon^{ij} + \hat{\lambda}\varepsilon^k_k\delta^{ij}.$$

Here the elastic moduli μ and λ are nonnegative because of the concavity of the entropy. By δ^{ij} we denote the Kronecker delta, the identity tensor with abstract index notation. A consequence of this calculation is that the Lamé coefficients are proportional to the density.

We have seen that specific quantities are the most straightforward starting points for constructing thermodynamic potentials in continua. In the following, we further develop this observation.

5. Thermostatistics of gradient elasticity with a gradient internal variable

The basic problem of using gradients of physical quantities as thermodynamic state variables is a shape dependence similar to that in case of deformation. After the previous considerations it is straightforward to introduce the necessary modifications and extend the elastic Gibbs relation. Now the specific entropy depends

on the internal energy, the strain gradient, $\partial_k \varepsilon^{ij}$, and an internal variable ξ^{ij} and its gradient $\partial_k \xi^{ij}$; therefore, $\mathbf{s} = \mathbf{s}(\mathbf{e}, \varepsilon^{ij}, \partial_k \varepsilon^{ij}, \xi^{ij}, \partial_k \xi^{ij})$. Let us denote the partial derivatives of the entropy as

$$\frac{\partial \mathbf{s}}{\partial \mathbf{e}} = \frac{1}{T}, \quad \frac{\partial \mathbf{s}}{\partial \varepsilon^{ij}} = -\mathbf{v} \frac{\sigma_{ij}}{T}, \quad \frac{\partial \mathbf{s}}{\partial (\partial_k \varepsilon^{ij})} = \mathbf{v} \frac{S_{ij}^k}{T}, \quad \frac{\partial \mathbf{s}}{\partial \xi^{ij}} = \mathbf{v} y_{ij}, \quad \frac{\partial \mathbf{s}}{\partial (\partial_k \xi^{ij})} = \mathbf{v} Y_{ij}^k.$$

The physical quantities here denoted by $S_{ij}^k, y_{ij}, Y_{ij}^k$ are particular intensive thermodynamic state functions in analogy with thermostatic terminology. We will see that some of the properties of usual intensive quantities are preserved. The corresponding Gibbs relation is written as

$$(5.1) \quad d\mathbf{e} = T d\mathbf{s} + \mathbf{v} \sigma_{ij} d\varepsilon^{ij} - \mathbf{v} S_{ij}^k d\partial_k \varepsilon^{ij} - \mathbf{v} T y_{ij} d\xi^{ij} - \mathbf{v} T Y_{ij}^k d\partial_k \xi^{ij}.$$

This will be our basic formula for the second law inequality and constructing a thermodynamic compatible evolution equation for ξ^{ij} and constitutive function for the stress and heat flux. The explicit appearance of temperature in the definition of the internal variable related intensive quantities is not fundamental, it expresses our traditional expectation that the strain directly contributes to the energy, as we have seen in (4.6), but the internal variable may influence the entropy more directly.

6. Entropy production of gradient elasticity with a weakly nonlocal internal variable

The entropy inequality is conditional. The fundamental balances are the conditions for the entropy inequality. In our case they are the conservation of mass, the conservation of momentum and the conservation of energy. The continuity equation for the conservation of mass is written as

$$(6.1) \quad \dot{\rho} + \rho \partial_i v^i = 0,$$

where the dot denotes the substantial, comoving time derivative, that is, $\dot{\rho} = \partial_t \rho + v^i \partial_i \rho$. By ∂_t and ∂_i we denote the partial time derivative and the gradient, respectively, and by v^i we denote the velocity field of the continuum, defined in the usual way as mass and momentum flow [82]. The balance of momentum is

$$\rho \dot{v}^i - \partial_j \tilde{\sigma}^{ij} = 0^i,$$

where $\tilde{\sigma}^{ij}$ is the stress tensor. The conservation of the moment of momentum is assumed; therefore, the stress is symmetric, $\tilde{\sigma}^{ij} = \tilde{\sigma}^{ji}$. Note that the stress in the momentum balance can be different from the static stress σ^{ij} , given as the derivative of the entropy function in (4.1) and for ideal elasticity in particular in (4.6). The balance of internal energy follows as (see, e.g. [32])

$$(6.2) \quad \rho \dot{e} + \partial_i q^i = \tilde{\sigma}^{ij} \partial_i v_j,$$

where q^i is the heat flux, the conductive current density of the internal energy. It is different from the energy flux $\hat{q}^i = q^i - \tilde{\sigma}^{ij} v_j$, the conductive current density of the total energy. The antisymmetric part of the velocity gradient tensor, which is the curl of the velocity field, does not play a role here, because of the symmetry of the stress.

The fourth condition that must be considered is the small strain version of the compatibility condition, that is,

$$(6.3) \quad \varepsilon^{ij} = \frac{1}{2}(\partial^i v^j + \partial^j v^i).$$

The substantial time derivative of the strain is the symmetric part of the velocity gradient.

The last condition is less evident, and it is the evolution equation of the internal variable, expressed explicitly as

$$\dot{\xi}^{ij} = f^{ij}(\mathbf{e}, \varepsilon^{ij}, \partial_k \varepsilon^{ij}, \xi^{ij}, \partial_k \xi^{ij}).$$

This condition expresses that the evolution equation of the internal variable is unknown and is to be determined constitutively, with the help of the second law. The restriction from the second law is universal, independent of the particular material structure which defines the internal variable, and this possibility is the most important consequence of recent thermodynamic investigations.

The entropy balance expresses the second law in the form of the following conditional inequality

$$\rho \dot{s} + \partial_i J^i = \Sigma \geq 0,$$

where the above conditions, (6.1)–(6.3), are to be considered in the simplest possible way, by direct substitution. Then the calculation of the entropy production is straightforward if the entropy flux is identified. For that purpose, the classical method of irreversible thermodynamics is applied [16]. The generalisation to the weakly nonlocal, gradient dependent case is straightforward, see, e.g. [5, 74]. The direct application of the Gibbs relation (5.1) requires using only the balance of the internal energy (6.2) and the compatibility condition (6.3). The balance of momentum is considered through the internal energy, and the continuity equation is not necessary because of the use of substantial derivatives and conductive fluxes. This simplification, common in fluid mechanics, considers comoving quantities, separating the changes in various fields due to the motion of the continuum from the changes of material origin. The whole procedure also the entropy production are absolute, reference frame and flow-frame independent. A more detailed explanation of the related objectivity issues was given in the introduction and [73]. The extension of those calculations for the present case is straightforward:

$$\begin{aligned} \rho \dot{s}(e, \varepsilon^{ij}, \partial_k \varepsilon^{ij}, \xi^{ij}, \partial_k \xi^{ij}) &= \frac{\rho \dot{e}}{T} - \frac{\rho}{\rho T} \sigma_{ij} \dot{\varepsilon}^{ij} + \frac{S_{ij}^k}{T} (\partial_k \varepsilon^{ij}) + y_{ij} \dot{\xi}^{ij} + Y_{ij}^k (\partial_k \xi^{ij}) \\ &= -\partial_k \left(\frac{q^k - S_{ij}^k \dot{\varepsilon}^{ij}}{T} - Y_{ij}^k \dot{\xi}^{ij} \right) + \partial_k \left(\frac{1}{T} \right) (q^k - S_{ij}^k \dot{\varepsilon}^{ij}) \\ &\quad - \frac{\dot{\varepsilon}^{ij}}{T} (\sigma^{ij} + \partial_k S^{kij}) + \frac{\partial_j v_i}{T} (\bar{\sigma}^{ij} - S_{kl}^j \partial^i \varepsilon^{kl} - T Y_{kl}^j \partial^i \xi^{kl}) \\ &\quad + f^{ij} (y_{ij} - \partial_k Y_{ij}^k) \geq 0. \end{aligned}$$

Here we can identify the entropy flux as $J^k = \frac{q^k - S_{ij}^k \dot{\varepsilon}^{ij} - T Y_{ij}^k \dot{\xi}^{ij}}{T}$, and a modified heat flux with an extra term $\hat{q}^k = q^k - S_{ij}^k \dot{\varepsilon}^{ij}$. Introducing the compatibility

condition, (6.3), one obtains for the entropy balance:

$$\begin{aligned} \rho \dot{s} + \partial_k \left(\frac{q^k - S_{ij}^k \dot{\varepsilon}^{ij} - TY_{ij}^k \dot{\xi}^{ij}}{T} \right) &= (q^k - S_{ij}^k \dot{\varepsilon}^{ij}) \partial_k \left(\frac{1}{T} \right) \\ &+ \frac{\dot{\varepsilon}^{ij}}{T} (\tilde{\sigma}^{(ij)} - \sigma^{ij} - \partial_k S^{kij} - S_{kl}^{(i} \partial^j) \varepsilon^{kl} - Y_{kl}^{(i} \partial^j) \xi^{kl}) \\ &+ \frac{\partial_{[j} v_{i]}}{T} (\tilde{\sigma}^{[ij]} - S_{kl}^{[j} \partial^i] \varepsilon^{kl} - TY_{kl}^{[j} \partial^i] \xi^{kl}) + f^{ij} (y_{ij} - \partial_k Y_{ij}^k) \geq 0. \end{aligned}$$

Here $(..)$ denotes the symmetric part of the corresponding tensorial components and $[..]$ denotes the antisymmetric one. In the calculation we used, the substantial and spatial derivatives do not commute, and the following identity was applied

$$(\partial_k \xi^{ij}) = \partial_k \dot{\xi}^{ij} - \partial_k v^l \partial_l \xi^{ij}.$$

Here $\sigma_{an}^{(ij)} = \tilde{\sigma}^{(ij)} - \sigma^{ij} - \partial_k S^{kij} - S_{kl}^{(i} \partial^j) \varepsilon^{kl} - Y_{kl}^{(i} \partial^j) \xi^{kl}$ is the symmetric *anelastic stress*. This expression is the extension of the usual viscous stress, $\sigma_{visc}^{ij} = \tilde{\sigma}^{ij} - \sigma^{ij}$. The additional anelastic terms are due to the internal variable and the gradient of the strain. We can see that weak nonlocality leads to couple-stresses both from the strain and internal variable gradients. We will call $\sigma_{an}^{[ij]} = \tilde{\sigma}^{[ij]} - S_{kl}^{[j} \partial^i] \varepsilon^{kl} - TY_{kl}^{[j} \partial^i] \xi^{kl}$ *anelastic couple-stress*.

The heat flux, \hat{q}^i , the dynamic stress, $\tilde{\sigma}^{ij}$, and the evolution equation of the internal variable, f^{ij} , are material dependent constitutive quantities. The entropy inequality determines their functional form. The simplest solution is to assume that \hat{q}^i , σ_{an}^{ij} and f^{ij} are linear functions of their multipliers in the entropy inequality, that is, we can introduce thermodynamic fluxes and forces, as shown in Table 1.

TABLE 1. Thermodynamic fluxes and forces of weakly nonlocal anelastic solids.

	Thermal	Mechanical	Couple	Internal
Fluxes	\hat{q}^i	$\sigma_{an}^{(ij)}$	$\sigma_{an}^{[ij]}$	f^{ij}
Forces	$\partial_i \left(\frac{1}{T} \right)$	$\frac{\dot{\varepsilon}^{ij}}{T}$	$\frac{\omega_{[ij]}}{T} = \frac{\partial_{[j} v_{i]}}{T}$	$y_{ij} - \partial_k Y_{ij}^k$

The identification of thermodynamic fluxes and forces must be based on their mathematical properties. Originally, for simple materials, thermodynamic forces have a gradient form, and thermodynamic fluxes are related to conductive current densities (called fluxes) of the balance form constraints [69]. In general, thermodynamic fluxes are to be related to constitutive functions, while thermodynamic forces are given operators, functions on the constitutive state space. Therefore, mechanical stress is not a force in a thermodynamical sense; it is a thermodynamic flux related to momentum transport in the material. From a physical point of view, thermodynamic fluxes are better considered characterising the deviation from local equilibrium and thermodynamic forces are to be considered as generalisations of gradients, their particular form being influenced by various constraints and the

structure of the state space. For example, in our case, the thermodynamic force for the internal interaction, related to the internal variable ξ^{ij} , is a complete partial functional derivative of the entropy density by the internal variable:

$$y_{ij} - \partial_k Y_{ij}^k = \rho \frac{\partial s}{\partial \xi^{ij}} - \partial_k \left(\rho \frac{\partial s}{\partial (\partial_k \xi^{ij})} \right) = \frac{\delta(\rho s)}{\delta \xi^{ij}}(\mathbf{e}, \varepsilon^{ij}, \partial_k \varepsilon^{ij}, \xi^{ij}, \partial_k \xi^{ij}).$$

Assuming that the constitutive functions are smooth and isotropic, the general solution to the entropy inequality follows from the Lagrange mean value theorem in the following form

$$\begin{aligned} \hat{q}^i &= \Lambda \partial_i \frac{1}{T}, \\ \sigma_{an}^{(ij)} &= l_{11} \varepsilon^{(ij)} + l_{12} (y_{(ij)} - \partial_k Y_{(ij)}^k) \\ (6.4) \quad \dot{\xi}^{(ij)} &= l_{21} \varepsilon^{(ij)} + l_{22} (y_{(ij)} - \partial_k Y_{(ij)}^k) \end{aligned}$$

$$\begin{aligned} (\sigma_{an})_k^k &= k_{11} \dot{\varepsilon}_k^k + k_{12} (y_k^k - \partial_l Y_k^{lk}) \\ (6.5) \quad \dot{\xi}_k^k &= k_{21} \dot{\varepsilon}_k^k + k_{22} (y_k^k - \partial_l Y_k^{lk}). \end{aligned}$$

$$\begin{aligned} \sigma_{an}^{[ij]} &= m_{11} \omega^{ij} + m_{12} (y_{[ij]} - \partial_k Y_{[ij]}^k) \\ (6.6) \quad \dot{\xi}^{[ij]} &= m_{21} \omega^{ij} + m_{22} (y_{[ij]} - \partial_k Y_{[ij]}^k). \end{aligned}$$

Here the representation theorems of isotropic functions were applied, that is, the second order spatial tensors were divided into a traceless symmetric, which is deviatoric, trace, which is spherical, and the antisymmetric parts as is customary in isotropic elasticity. Some of the material coefficients are well known. By $\Lambda_F = \Lambda/T^2$ we denote the Fourier heat conductivity coefficient, and l_{11} and k_{11} are the linear viscoelastic coefficients of a Kelvin–Voigt body. The second law nonnegativity of the entropy production requires the positive definiteness of the symmetric parts of the coefficient matrices and therefore the following sign restrictions follow:

$$\begin{aligned} \Lambda, l_{11}, l_{22}, k_{11}, k_{22}, m_{11}, m_{22} &\geq 0, \\ (6.7) \quad l_{11} l_{22} - \frac{l_{12} + l_{21}}{4} &\geq 0, \quad k_{11} k_{22} - \frac{k_{12} + k_{21}}{4} \geq 0, \quad m_{11} m_{22} - \frac{m_{12} + m_{21}}{4} \geq 0. \end{aligned}$$

Equations (6.4) and (6.5) are the weakly nonlocal generalisation of the Kluitenberg–Verhás body [3], the fundamental building block of thermodynamic rheology. The difference is that here the thermodynamic forces and fluxes are gradient dependent. It is important to remark that the symmetry of the Onsagerian coefficient matrices cannot be required; therefore, $l_{12} \neq l_{21}$, $k_{12} \neq k_{21}$, $m_{12} \neq m_{21}$ in general, as is experimentally observed in case of rock materials for the deviatoric and spherical parts [41, 45, 46]. The coefficients are not necessarily constant, they may be state dependent, and, in general, in a fully nonlinear case, they may depend on the thermodynamic forces, too.

6.1. Ideal anelastic materials. It is worth inspecting an important special case of our continuum model, when the material is not dissipative. There are several distinct possibilities. Let us assume now that the internal thermodynamic force, $y_{ij} - \partial_k Y_{ij}^k$, heat flux and the anelastic stress are zero. Then the following constitutive functions and field equations are to be considered:

$$(6.8) \quad q^k = S_{ij}^k \varepsilon^{ij},$$

$$\bar{\sigma}^{ij} = \sigma^{ij} + \partial_k S^{kij} + S_{kl}^i \partial^j \varepsilon^{kl} + TY_{kl}^i \partial^j \xi^{kl}$$

$$(6.9) \quad 0 = \rho \frac{\partial s}{\partial \xi^{ij}} - \partial_k \left(\rho \frac{\partial s}{\partial (\partial_k \xi^{ij})} \right) = \frac{\delta(\rho s)}{\delta \xi^{ij}}.$$

In this case the continuum is not necessarily at rest, the rate of the strain is not necessarily zero, as one can see from the constitutive equations (6.4)–(6.6) above.

A remarkable consequence of the fact that the heat flux is not zero is that by substituting (6.8) into the balance of internal energy one can see the propagation of internal energy connected to the strain changes, that is,

$$\rho \dot{e} + \partial_k (S_{ij}^k \dot{\varepsilon}^{ij}) = 0.$$

The internal energy is conserved because the mechanical power is zero. However, the momentum balance has the following form:

$$(6.10) \quad \rho \dot{v}^i - \partial_j (\sigma^{ij} + \partial_k S^{kij} + S_{kl}^i \partial^j \varepsilon^{kl} + TY_{kl}^i \partial^j \xi^{kl}) = 0.$$

Moreover, considering (6.9) the internal variable related stress term can be converted to force density and the equation transforms to

$$(6.11) \quad \rho \dot{v}^i - \partial_j (\sigma^{ij} + \partial_k S^{kij} + S_{kl}^i \partial^j \varepsilon^{kl}) = -\rho \nabla_{\xi}^i s.$$

Here $\nabla_{\xi} s = \partial_{\xi^{kl}} s \partial^i \xi^{kl} + \partial_{(\partial_j \xi^{kl})} s \partial_j^i \xi^{kl}$, the partial gradient of the specific entropy, due to the internal variable. If the entropy is additively decomposed into strain and internal variable dependent parts, that is, $s(\mathbf{e}, \varepsilon^{ij}, \partial_k \varepsilon^{ij}, \xi^{ij}, \partial_k \xi^{ij}) = s_{ela}(\mathbf{e}, \varepsilon^{ij}, \partial_k \varepsilon^{ij}) + s_{int}(\xi^{ij}, \partial_k \xi^{ij})$, then the gradient of the second part, s_{int} , is a force density because $\nabla_{\xi}^i s = \partial_i s_{int}$.

7. Concluding remarks: internal variables, phase fields and gravitation

Finally, we offer some general remarks.

- It is remarkable that according to the continuity equation and the compatibility condition, (6.3) and (6.1), the density and the strain are not independent, because: $\frac{\dot{\rho}}{\rho} = \dot{\varepsilon}_i^i$. Therefore, $\varepsilon_i^i = \ln \frac{\rho}{\rho_0}$, where ρ_0 is constant. However, thermostatics, with the definition of state variables and thermodynamic potentials, precedes the calculation of entropy production, and the continuity equation is a constraint there.
- The results of these heuristic calculations can be obtained with more rigorous methods, too. Regarding objectivity, see [24], where it was shown that our framework—that is a first-order weakly nonlocal constitutive state space with balance constraints—leads to the classical form of entropy production.

- Sometimes it is assumed that a gradient itself can be an internal variable (see, e.g. [5, 80]). Here it is shown that it can be misleading because surface and bulk contributions differ, and evolution equation and boundary conditions are affected.
- In a finite deformation framework, natural objective derivatives, such as Lie derivatives, appear in the evolution of the internal variable (see, e.g. [71]). Also, spatial interactions are influenced [6]. Our treatment here did not introduce material manifolds, which should be a logical next step in this research.

The most remarkable aspect of our treatment is the stress force relation of the ideal solid, expressed in (6.10) and (6.11). According to the constitutive relations (6.4)–(6.6) and in particular the sign restrictions of (6.7), the evolution of the internal variable is relaxational and eventually becomes static. The developed static structure satisfies (6.9). This behaviour is general, and it is independent of the tensorial properties of the internal variable. Then the internal variable related stresses are bulk, and all stress contributions may appear as force density in the momentum balance. This is a natural, *dynamic homogenisation* process.

We have mentioned that, without the gradient contributions and couple-stresses, our treatment is reduced to the Kluitenberg–Verhás rheological body [3, 25, 64, 79]. However, the previous considerations open up the possibility to generalise the constitutive framework of continuum mechanics into various directions together with the constructive approach of nonequilibrium thermodynamics. Weakly nonlocal extension of the classical state variables, memory effects with internal variables and the combination of memory effects and gradient effects offer a rich framework of material modelling. For example, the previously mentioned stress-force relation for static internal variables shows the natural connection of microforce balance based material models [23, 28, 31], and theories with internal variables. The extension considering spatial nonlocalities of the internal variables in a higher-order weakly nonlocal state spaces leads to phase field theories [74, 76]. Introducing a second tensorial internal variable leads to dual internal variables and results in the micromorphic theory [5, 81].

The generalisation of the Fourier law, the heat conduction theory, is also straightforward. It leads to experimentally confirmed effects in complex materials at room temperature [8, 82]. The connection between mechanical and thermal effects in this framework of nonequilibrium thermodynamics is a source of experimental and technological predictions [35].

Finally, I would like to mention one of the most striking consequences of the internal variable approach, highlighting the importance of the fine details of weak nonlocality and the requirement of extensivity. Let us assume that a part of the internal energy is weakly nonlocal with a square gradient weak nonlocality with the following Gibbs relation:

$$du = Tds - pdv = de - d\varphi - d\left(\frac{\partial^i \varphi \partial_i \varphi}{8\pi G\rho}\right).$$

With the previous methods of nonequilibrium thermodynamics, it is easy to show that ϕ is the Newtonian gravitational potential and we obtain a dissipative theory of gravity, which in the ideal case reduces to the usual one, where the field equation for the gravitational potential ϕ is the Poisson equation: $\partial_i^2 \phi = 4\phi G\rho$. However, the general nondissipative dynamics is more general and also reproduces the field equations of Modified Newtonian Dynamics (MOND) [77].

Acknowledgments. The work was supported by the grants of the National Research, Development and Innovation Office - NKFIH 124366 (124508), 123815, TUDFO/ 51757/2019-ITM (Thematic Excellence Program) and FIEK-16-1-2016-0007. The research reported in this paper was supported by the Higher Education Excellence Program of the Ministry of Human Capacities within the framework of the Nanotechnology research area of the Budapest University of Technology and Economics (BME FIKP-NANO). The author thanks Robert Kovács for valuable discussions.

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**ТЕРМОДИНАМИЧКИ КОНЗИСТЕНТНА ГРАДИЈЕНТНА
ЕЛАСТИЧНОСТ СА УНУТРАШЊОМ ПРОМЕНЉИВОМ**

РЕЗИМЕ. Улога термодинамике у механици континуума и извођење одговарајућих конститутивних односа је важна проблематика у Рационалној механици. Класични радови мало су се ослањали на добијене резултате о термостатацима и били су веома критични према хеуристичким методама преверзибилне термодинамике. У овом раду је заснована теорија еластичности градијента малих деформација са ефектима памћења и дисипацијом. То је метода нееквilibријумске термодинамике са унутрашњим променљивим; према томе, конститутивни односи су по конструкцији компатибилни са термодинамиком. Уводе се термостатске Гибсове релације за еластична тела са једном тензорском унутрашњом променљивом. Термодинамички потенцијали су првог реда слабо нелокални и израчунава се производња ентропије. Затим се конструишу конститутивне функције и еволуциона једначина унутрашње променљиве. Анализа другог закона показала је допринос, такође без дисипације, градијентних чланова у напону.

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(Received 04.02.2020.)

(Revised 27.05.2020.)

(Available online 11.06.2020.)