

INTERNAL VARIABLES IN THERMOELASTICITY

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1 Introduction

Two well established theories exist for the description of macroscopic behavior of materials: classical equilibrium thermodynamics and classical (linear) continuum mechanics. Both theories have a good experimental and methodological foundation, they are mathematically correct and represented in different equivalent forms. The only inconvenient thing is that these theories are highly idealized approximations of real processes in materials. Advanced materials like polymers, composite materials, biomaterials, etc. are, as a rule, inhomogeneous. Their inner structure depends on a fabrication method and cannot be taken into account in detail. The use of such materials in practice requires the knowledge of the influence of the inner structure on the behavior of materials. The exact description is impossible or at least tedious: any refinement is only an approximation. The question is in the built-in information about the material structure.

It is well understood that idealized classical theories are not sufficient for inhomogeneous microstructured materials. The accuracy in the prediction of the material behavior depends on the chosen theoretical description. The complete atomistic exposition is possible only in principle, and in any case it is difficult for using in practice. The compromise between the full accuracy and a practical treatment can be achieved in various ways. One of such possibilities is presented in this paper.

2 Internal variables

The considered approach supposes the introduction of internal variables to characterize the influence of a microstructure on the global behavior of a material. This idea is not new and has been exploited at least for 50 years. It was broadly applied in rheology, plasticity, and phase-field theory. However, its full power has been uncovered only recently. The use of the internal variable concept in a more extended context, i.e., the introduction of dual internal variables, provides an unified treatment both of internal variables of state and of dynamic degrees of freedom. This extension covers both parabolic evolution equations for dissipative internal variables and hyperbolic evolution equations in the absence of dissipation. Both forms of evolution equations follow from the dissipation inequality, and, therefore, are thermodynamically consistent. The structure of well known evolution equations for the Cosserat microrotation and for the micromorphic microdeformation is recovered in the framework of the proposed approach in the non-dissipative limit. In the case of heat conduction, an evolution equation for the microtemperature is obtained by keeping the coupled parabolic equation for the global temperature.

3 Thermoelasticity

The purpose of thermoelasticity is the prediction of the response of a body to an external mechanical or thermal loading. If the body is considered as an elastic one, then its isothermal response is governed by the Hooke law. The model of the elastic body is the simplest model of material behavior. On the other hand, the thermal response of a rigid body can be described by the Fourier law (again in the simplest case). It should be emphasized that these simple models have distinct mathematical structures. The description of the dynamics of an elastic body includes a second-order time derivative in the equation of motion presented in terms of displacement. Such an equation is a hyperbolic partial differential equation. The Fourier law, in its turn, provides the heat conduction equation with the first-order time derivative for temperature. Mathematically, the latter is a parabolic partial differential equation. Coupling of elastic and thermal effects results in the thermoelasticity theory for homogeneous bodies.

4 Microstructure

In reality, all bodies are inhomogeneous, excluding perfect crystals and artificially refined materials. Usually materials possess a microstructure characterized by various size, distribution, and properties of inclusions or imperfections. Although the length scale of the microstructure is, as a rule, much smaller than the length scale of a body, the impact of microstructure on overall response of the body may not be necessarily small. The demand of accounting of the influence of microstructure dictates the improvement of macroscopic material theories.

There exists several directions in the description of the microstructure influence. The first one is micromechanics, which serves for the determination of properties of "effective" media by homogenization methods [1,2]. The homogenized "effective" medium is used then instead of the original microstructured material for the prediction of its thermomechanical response. The homogenization methods of micromechanics are well suited for static problems with periodic or statistically homogeneous distribution of inhomogeneities.

The second approach introduces memory and nonlocal effects in the model, either using memory functionals and nonlocal kernels (strong nonlocality) or higher order time and space derivatives (weak nonlocality) [3]. Gradient models with nonlocality in space are typical examples of the latter method. A particular theoretical method of this family is GENERIC [4].

The third approach corresponds to generalized continuum theories. A number of advanced generalized continuum theories have been introduced over the past five decades to take into account the influence of the structural inhomogeneities on the macroscopic behavior of materials. In general terms, such theories include coarse grained morphological descriptors to describe the morphology of the material element [5,6]. The morphological descriptors represent certain additional independent kinematic fields. The most known example of the morphological descriptor is the microrotation vector in the Cosserat material. Another example is the second order symmetric tensor of microdeformation introduced by Mindlin [7], who considered the material element as a cell able to deform independently of the rest of the body. The relevant continuum theory is called micromorphic [8]. The micromorphic theory is the most successful top-down formulation of a two-level continuum model, in which the overall deformation is composed of the macroscopic continuous deformation and the internal microscopic deformation of the inner structure.

The distinction between homogenization methods, nonlocal and generalized continuum theories is not sharp. Generalized continua are probably the most flexible: morphological descriptors can be obtained by homogenization [8] and may have certain weak or strong nonlocality. The separation of the macro- and micromotion in generalized continuum theories needs to postulate separate balance laws at the macro- and the micro- levels, like in [7]. Then the suitable boundary conditions are required as well.

5 Thermodynamics with internal variables

It is clear that material elements in generalized continuum theories extend the classical thermodynamic state space beyond equilibrium one. This dictates to choose the method of the description of such non-equilibrium states, especially in the presence of dissipative processes. The classical theory of irreversible processes (TIP) is not sufficient for such a description because its basic hypothesis is the local thermodynamic equilibrium. The choice of an appropriate thermodynamical description is essential. Among several versions of non-equilibrium thermodynamics, the *thermodynamics with internal variables (TIV)* holds a specific place. This theory (TIV) is the direct extension of TIP beyond local equilibrium. We chose the thermodynamics with internal variables because it does not introduce any assumption about the physical mechanism of the modelled phenomenon in advance and, therefore, can be developed in an universal form. Moreover, it assumes the strict validity of thermodynamic concepts also for the internal variables. This way we insist the most conservative use of thermodynamics outside local equilibrium.

6 Internal variables of state and dynamic degrees of freedom

There exist two basic methods to generate the evolution equations for internal variables. Both methods are based on fundamental principles. The *first method* generates the evolution equations exploiting the entropy inequality. This approach uses exclusively thermodynamic laws, and the corresponding variables are called *internal variables of state*. This framework has the advantage of operating with familiar thermodynamic concepts like thermodynamic force and entropy, however, no inertial effects are considered. Internal variables of state are usually introduced in the case of dissipative processes. They must satisfy only the second law of thermodynamics, and need not be balanced. The dissipation (or internal power) induced by an internal variable of state is equal to the product of its rate of change and the corresponding conjugated force [9]. Accordingly, the evolution equation includes only first-order time derivative of the internal variable. In the internal variable theory, a concept of a local constrained non-equilibrium state is introduced. In other words, there always exists a local accompanying equilibrium (or quasi-equilibrium) state, onto which the local non-equilibrium state can be projected [10]. Internal variables add extra dimensions to the thermodynamic state space.

The *second method* constructs the evolution equations through a Hamiltonian variational principle and therefore inertial effects are unavoidable. This approach has a mechanical flavor, and the corresponding variables are called *internal degrees of freedom*. Dissipation in this case is added by dissipation potentials. This theoretical frame has the advantage of operating with familiar mechanical concepts, like force and energy. Internal degrees of freedom are endowed with both inertia and flux, where the latter is not necessarily purely dissipative (on the contrary, it could be purely non-dissipative) [9]. The corresponding evolution equations contain the second-order time derivatives of the dynamic degrees of freedom.

Both internal variables of state and internal degrees of freedom are used to take into account the influence of internal processes on the global behavior of materials. Both of them are introduced in addition to classical field quantities. However, the differences in the approaches are much larger. Internal variable of state is characterized by:

- the extension of the thermodynamic state space; the extended entropy function should be concave,
- the calculation of the entropy production accounting the internal energy balance and the evolution equation of the internal variable,
- the solution of the dissipation inequality providing properly introduced constitutive functions; usually a linear solution is good enough.

In its turn, the main features for the dynamic degree of freedom are:

- the thermodynamic state space is not extended,
- evolution equation for a dynamic degree of freedom is determined by the choice of a Lagrangian and the independent choice of a dissipation potential.

Both theories can have a weakly nonlocal extension. In that case natural boundary conditions can be calculated by variational means in the case of dynamics degrees of freedom and by the zero entropy flux prescription at boundaries in the case of internal variables. The most important difference between the two approaches consists in the parabolicity of evolution equations for internal variables of state and hyperbolicity of balance laws for the dynamic degrees of freedom. It is also important to observe that internal degrees of freedom need the variational method and thermodynamic relations simultaneously, whereas for internal variables of state there is no need anything beyond thermodynamics.

7 Dual internal variables

Let us fix the state of the art. There exist two clearly distinctive types of internal variables: internal degrees of freedom and internal variables of state [9]. By definition, internal variables of state must have no inertia, and they produce no external work. The internal variables of state are not governed by a field equation, i.e., by their own balance law; the power expended by internal variables will be only of the dissipative type. On the contrary, the internal degrees of freedom obey their own balance law. Both internal degrees of freedom and internal variables of state are introduced to capture microstructural properties in a macroscopic description. The thorough thermomechanical theory with weakly nonlocal internal variables of state is presented recently by Maugin [11]. It can be called as a *single internal variable* theory. In the case of internal degrees of freedom the complete description is not finished yet. This is why "a unified continuum mechanical description of materials with inherent microstructure is to date not available" [12].

The introduction of any kind of internal variables should be in the correspondence with the second law of thermodynamics. The latter indicates the direction for an unified continual description of materials with microstructure. The main idea is that one can obtain the form of the evolution equation and also the connection to other processes, considering only basic principles, first of all, the second law of thermodynamics. Evolution equations derived from any structural, mesoscopic, or microscopic realization of the extra field variable must belong to this general form, as long as they are restricted by the same basic principles.

We propose a uniform approach based exclusively on thermodynamic laws. Our suggestion requires dual internal variables and a generalization of the usual postulates of non-equilibrium thermodynamics: we do not require the satisfaction of the Onsagerian reciprocity relations. With dual internal variables we are able to include inertial effects and to reproduce the evolution of dynamic degrees of freedom. In other words, instead of the doubling of the theoretical structure we suggest the doubling of the number of internal variables.

In spite of the fine details where these notions are different for various authors (controllability, boundary conditions, weak nonlocality, etc.), we can find a sufficiently general framework where these concepts are combined. This framework appears to be a powerful modelling tool of modern continuum physics [13,14]. In what follows, we will demonstrate the constructive modelling power of this conceptual framework.

As long as evolution equations of internal variables are determined by basic macroscopic principles, we can expect that the validity of the evolution equations is independent of particular microscopic models. The method of internal variables can be considered as a universal modelling tool for macroscopic field theories. It based on minimal number of assumptions about the physical mechanism of the modelled phenomena.

8 Conclusions

The prediction of the response of a material (or a structure) to external loading is an ordinary engineering problem. It is a necessary step in the design of any man-made tools, devices, and constructions. Increasing complexity of advanced electronics, modern machinery and equipment, and of corresponding materials demands more and more sophisticated methods for their proper handling.

The thermoelastic theory with internal variables provides a general framework for the prediction of a material reaction on an external loading [13]. If classical elasticity theory can be considered as non-dispersive and non-dissipative, then the introduction of an internal variable of state makes the corresponding theory non-dispersive, but dissipative [9]. The insertion of an internal degree of freedom instead of an internal variable of state leads to a dispersive but non-dissipative theory. The dual internal variables concept allows to consider internal variables of state and internal degrees of freedom as specific cases in the unified formalism [13]. The respective weakly nonlocal theory is both dispersive and dissipative [15].

It should be noted that dual internal variables generate different thermodynamic forces for microdeformation and for microtemperature [16]. In the simplest case this results in the hyperbolicity of equations of motion both at micro- and macro- levels in the case of the microdeformation in the nondissipative limit of the general dissipative theory, while a hyperbolic evolution equation for the microtemperature is complemented by a parabolic heat conduction equation for the macrotemperature [14]. The distinction between thermal and mechanical processes is emphasized by the introduction double dual internal variables. This means that independent dual internal variables are introduced for the description of thermal and mechanical effects [17].

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