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An incremental variational approach to coupled thermo-mechanical problems in anelastic solids. Application to shape-memory alloys

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ABSTRACT

We study the coupled thermo-mechanical problem that is obtained by combining generalized standard materials with Fourier's law for heat conduction. The analysis is conducted in the framework of non-smooth mechanics in order to account for possible constraints on the state variables. This allows models of damage and phase-transformation to be included in the analysis. In view of performing numerical simulations, an incremental thermo-mechanical problem and corresponding variational principles are introduced. Conditions for existence of solutions to the incremental problem are discussed and compared with the isothermal case. The numerical implementation of the proposed approach is studied in detail. In particular, it is shown that the incremental thermo-mechanical problem can be recast as a concave maximization problem and ultimately amounts to solve a sequence of linear thermal problems and purely mechanical (i.e. at a prescribed temperature field) problems. Therefore, using the proposed approach, thermo-mechanical coupling can be implemented with low additional complexity compared to the isothermal case, while still relying on a sound mathematical framework. As an application, thermo-mechanical coupling in shape memory alloys is studied. The influence of the loading strain-rate on the phase transformation and on the overall stress–strain response is investigated, as well as the influence of the thermal boundary conditions. The numerical results obtained by the proposed approach are compared with numerical and experimental results from the literature.

1. Introduction

This paper focuses on coupled thermo-mechanical evolutions of dissipative solids, in the geometrically linear (small strains) setting. The framework of generalized standard materials in non-smooth mechanics is considered (Halphen and Nguyen, 1975; Moreau and Panagiotopoulos, 1988; Frémond, 2002). In that framework, the local state of the material is described by the strain $\boldsymbol{\varepsilon}$, the temperature θ, and an internal variable $\boldsymbol{\alpha}$. The constitutive laws are determined from the Helmholtz free energy w and a convex dissipation potential Φ. In its original form (Halphen and Nguyen, 1975), that framework covers a wide range of elasto–plastic models, including limited and nonlinear hardening. Its extension to non-smooth mechanics has been extensively studied by Frémond (2002) and allows constraints on the internal variable $\boldsymbol{\alpha}$ to be taken into account in a rigorous fashion. That feature is crucial for the modelling of such phenomena as damage or phase-transformation, as the internal variable in such cases is typically bounded. The thermodynamic analysis of the media considered is presented in Section 2, leading to a boundary value problem for the mechanical and thermal fields. As pointed out by Yang et al. (2006), the time-discretization of the thermo-mechanical evolution problem is a sensitive issue because of the coupling between mechanical and thermal equations. For instance, the Euler implicit scheme leads to an incremental thermo-mechanical problem for which existence of solutions cannot generally be ensured. This is in contrast with the isothermal case, for which the Euler implicit scheme provides a well-posed incremental problem under standard assumptions of convexity on the functions w and Φ.

One objective of this paper is to propose a sound time-discretization scheme for coupled thermo-mechanical problems, retaining some essential features displayed by the Euler scheme in the isothermal case (most notably the consistency with the rate problem and the existence of solutions). A central idea is the use of a variational formulation for the incremental problem. Incremental variational principles for dissipative solids have been the focus of a lot of attention in recent years, offering new perspectives in various topics such as finite-strains elasto-viscoplasticity (Ortiz and Stainier, 1999), homogenization (Miehe, 2002; Lahellec and Suquet, 2007), formation and stability of microstructures (Ortiz and Repetto, 1999; Miehe et al., 2004). Incremental variational principles for coupled thermo-mechanical problems have been proposed by Yang et al. (2006) in the case where the heat flux $\boldsymbol{q}$

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derives from a potential χ in $(\nabla\theta)/\theta$, i.e. when the heat conduction law takes the form $\boldsymbol{q} = -\chi'((\nabla\theta)/\theta)$. In this paper, we stick with the standard Fourier's law of heat conduction $\boldsymbol{q} = -K\nabla\theta$, which does not fall in the format considered by Yang et al. (2006).

In Section 3 we introduce an incremental problem for the class of coupled thermo-mechanical problems considered, along with a corresponding variational formulation. The variational formulation of the incremental thermo-mechanical problem serves two purposes. First, it allows the existence of solutions to be studied, as discussed in Section 3. Second, the variational formulation leads to a convenient and efficient way of solving the incremental thermo-mechanical problem. The latter can be indeed be recast as a concave maximization problem, for which well-known algorithms are available. As detailed in Section 4, an advantage of that approach is that the solution of the thermo-mechanical problem can be obtained by solving a sequence of linear thermal problems and purely mechanical (i.e. at prescribed temperature) problems. This calls for an easy implementation in an existing finite-element code. A crucial point in the analysis lies in the introduction of an auxiliary linear problem, akin to the adjoint state used in optimal control problems (Lions, 1968).

As an application, the proposed method is used in Section 5 to study thermo-mechanical coupling in shape-memory alloys. The significant role of thermal effects in shape-memory alloys has notably been put forward by Peyroux et al. (1998) and Chrysochoos et al. (2003). The solid/solid phase transformation that occurs in those materials is known to produce significant amounts of heat, associated both with recoverable latent heat effects and irreversible frictional contributions. Depending on the rate of loading and on the thermal exchange conditions, the heat produced by the phase transformation may not have time to diffuse in the body and the temperature field may become inhomogeneous. In such conditions, the overall stress–strain response becomes significantly different from its isothermal counterpart, and it is mandatory to take the thermo-mechanical coupling into account. Therefore, shape-memory alloys offer a particularly relevant application of the general methods presented in this paper. In Section 5, the influence of thermal effects on the phase-transformation and on the overall stress–strain curve is investigated in detail.

2. Thermo-mechanical evolutions of continuous media

2.1. Thermodynamic principles

Consider the evolution (on a time interval $[0,T]$) of a continuous medium occupying a domain Ω in the reference configuration. We restrict our attention to the geometrically linear setting, defining the strain $\boldsymbol{\varepsilon}$ as $\boldsymbol{\varepsilon} = 1/2(\nabla\boldsymbol{u} + \nabla^T\boldsymbol{u})$ where $\boldsymbol{u}$ is the displacement. The first principle of thermodynamics gives

$$\int_t^{t'} \dot{E}d\tau + \int_t^{t'} \dot{K}d\tau = \int_t^{t'} Pd\tau + \int_t^{t'} \mathring{Q}dt \text{ for all } 0 \leqslant t \leqslant t' \leqslant T. \quad (1)$$

In Eq. (1), K and E are respectively the kinetic and the internal energy of the system. The internal energy E can be written in the form $E = \int_\Omega e d\boldsymbol{x}$ where e is the internal energy density. In the right-hand side of (1), P denotes the power of external loads, and $\mathring{Q}$ is the rate of heat received by the system. The upper dot in (1) denotes left-time derivative.[1] The principle of virtual power gives the relation

$$\dot{K} = P - \int_\Omega \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} d\omega \quad (2)$$

where $\boldsymbol{\sigma}$ is the stress. Expressing $\mathring{Q}$ as

$$\mathring{Q} = -\int_{\partial\Omega} \boldsymbol{q}.\boldsymbol{n} d\omega + \int_\Omega r d\omega \quad (3)$$

where $\boldsymbol{q}$ is the heat flux and r a heat source, the relation (1) can be rewritten as

$$\int_t^{t'} \int_\Omega (\dot{e} - \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + \operatorname{div}\boldsymbol{q} - r)\, d\omega d\tau = 0 \text{ for all } 0 \leqslant t \leqslant t' \leqslant T. \quad (4)$$

The relation (4) also holds when replacing Ω with an arbitrary subdomain $\Omega' \subset \Omega$. Therefore, we obtain the local equation

$$\dot{e} - \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + \operatorname{div}\boldsymbol{q} - r = 0 \text{ a.e. in } \Omega \times [0,T] \quad (5)$$

where the abbreviation 'a.e' stands for 'almost everywhere'. The second principle of thermodynamics gives

$$\int_t^{t'} \int_\Omega \dot{s}\, d\omega d\tau \geqslant \int_t^{t'} \int_\Omega \frac{r}{\theta} - \operatorname{div}\frac{\boldsymbol{q}}{\theta}\, d\omega d\tau$$

where s is the entropy density and θ is the local temperature. Using a similar reasoning as above, we obtain the relation

$$\theta\dot{s} - r + \operatorname{div}\boldsymbol{q} - \boldsymbol{q}.\frac{\nabla\theta}{\theta} \geqslant 0 \text{ a.e. in } \Omega \times [0,T].$$

Making the classical assumption of separation between the intrinsic dissipation $\theta\dot{s} - r + \operatorname{div}\boldsymbol{q}$ and the thermal dissipation $-\boldsymbol{q}.(\nabla\theta)/\theta$, we obtain the inequalities $-\boldsymbol{q}.(\nabla\theta)/\theta \geqslant 0$ and

$$\theta\dot{s} - r + \operatorname{div}\boldsymbol{q} \geqslant 0 \text{ a.e. in } \Omega \times [0,T]. \quad (6)$$

Eqs. (5),(6) can be rewritten in terms of the Helmholtz free energy density $w = e - \theta s$ as

$$\dot{w} + \theta\dot{s} + s\dot{\theta} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + r - \operatorname{div}\boldsymbol{q} \text{ a.e. in } \Omega \times [0,T], \quad (7)$$

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - s\dot{\theta} - \dot{w} \geqslant 0 \text{ a.e. in } \Omega \times [0,T]. \quad (8)$$

2.2. Mechanical constitutive laws

In the framework of standard generalized materials (Halphen and Nguyen, 1975), the local state of the material is described by the strain $\boldsymbol{\varepsilon}$, the temperature θ, and an internal variable $\boldsymbol{\alpha}$ living in a vectorial space denoted by $\mathbb{A}$. The constitutive laws are determined by the Helmholtz free energy $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \theta)$ and a convex dissipation potential $\Phi(\dot{\boldsymbol{\alpha}})$ according to the following relations:

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}, \quad (9.1)$$

$$\boldsymbol{A} = -\frac{\partial w}{\partial \boldsymbol{\alpha}}, \quad (9.2)$$

$$s = -\frac{\partial w}{\partial \theta}, \quad (9.3)$$

$$\boldsymbol{A} \in \partial\Phi(\dot{\boldsymbol{\alpha}}), \quad (9.4)$$

where ∂ denotes the subdifferential operator. Recall (Brézis, 1972) that the subdifferential ∂f of a function $f : \mathbb{A} \mapsto \mathbb{R}$ is the multi-valued mapping defined by

$$\partial f(\boldsymbol{x}) = \{\boldsymbol{\tau} \in \mathbb{A} | f(\boldsymbol{y}) - f(\boldsymbol{x}) \geqslant \boldsymbol{\tau}.(\boldsymbol{y} - \boldsymbol{x})\ \forall \boldsymbol{y} \in \mathbb{A}\}. \quad (10)$$

In the following, the dissipative behaviour is assumed to be *rate-independent*. In such case, the dissipation potential Φ is positively homogeneous of degree 1, i.e. satisfies

$$\Phi(\lambda\dot{\boldsymbol{\alpha}}) = \lambda\Phi(\dot{\boldsymbol{\alpha}}) \text{ for any } \lambda \in \mathbb{R}^+ \text{ and } \dot{\boldsymbol{\alpha}} \in \mathbb{A}. \quad (11)$$

[1] In non-smooth mechanics, left- and right-time derivative of physical quantities may not be equal. In order to respect the principle of causality, the constitutive relations need to be written in terms of left-time derivatives (see e.g. Frémond, 2002).