

## VARIATIONAL CONSTITUTIVE UPDATES FOR A FULLY COUPLED THERMO-MECHANICAL PROBLEM

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**Abstract.** *The total separation of mechanical and thermal effects is a reasonable assumption for most applications in solid mechanics. However, some problems require more complex models. Glass transition temperatures for rubber-like polymers and everyday experience with thermal softening of plastics constitute evidence of the need for considering thermo-mechanical coupling, when dealing with these materials. Even metals, when subjected to large strains or strain rates, exhibit macroscopic heating effects. The clear need for coupled thermo-mechanical models has led to the extensive study of such effects as thermal stresses and thermoelastic heating and cooling for a wide range of materials and applications. The aim of this paper is to formulate a fully coupled thermo-mechanical problem in a variational structure, considering isotropic hyperelastic-viscoplastic materials. The construction of an incremental pseudo-potential leads to the computation of constitutive updates. More specifically, an adiabatic problem is considered. For simplicity reasons, no local heat generation or heat flux are considered in this paper, which allows the temperature to be considered as an additional internal variable. The local heat balance problem is derived from the coupled thermo-mechanical potential, along with equations describing the mechanical part of the problem. Temperature dependence is briefly discussed for all the potentials used in the construction of the incremental pseudo-potential. The resulting non-linear problem with respect to temperature and cumulated plastic strain is solved, allowing for the prediction of temperature increase and heat dissipation during deformation, as well as a correct description of mechanical behavior influenced by thermal fields. A comparison to experimental results for selected materials found in literature is presented.*

**Keywords:** *thermo-mechanical coupling, variational formulation, constitutive updates.*

### 1. INTRODUCTION

The application of variational principles for dissipative mechanical systems has been the theme of many recent papers. Ortiz and Stainier (1999) developed variational constitutive updates for a rather general range of material models, including irreversible, dissipative and rate-dependent behaviors. The works of Fancello *et al.* (2006), with application to nonlinear finite viscoelasticity problems, and Fancello *et al.* (2008), extending the approach of the previous paper to finite isotropic viscoplasticity, base the construction of constitutive updates on the use of spectral quantities of independent variables. This allowed for the adoption of a wider variety of potentials within the same formalism.

Owing to the need to consider thermal effects in many contexts, the study of thermo-mechanically coupled formulations has also been of recent interest. Yang *et al.* (2006) and Stainier and Ortiz (2008) list a number of fields of application where the assumption of mechanical behavior independent of thermal effects proves to be insufficient. In such diverse applications such as metal forming and ballistic penetration, common characteristics such as high strain rates and heat dissipation due to plastification indicate the conditions that motivate the construction of coupled thermo-mechanical models for dissipative materials.

The aim of the present paper is to extend the formulation used by Fancello *et al.* (2008) to an adiabatic fully-coupled thermo-viscoplastic model. Potentials based on spectral quantities are used in order to allow for more versatility. By considering the problem to be adiabatic (a reasonable hypothesis when the time range under consideration is short, according to Stainier and Ortiz (2008)), thermal effects can be treated locally, and temperature becomes an internal variable.

Section 2 presents briefly the form of a general incremental pseudo-potential for a purely mechanical dissipative problem, as an inspiration for our thermally coupled model. Section 3 then proceeds to show the steps necessary to make the extension of the model. After some preliminary definitions and hypotheses (Sect.3.1.), we explore thermodynamic aspects (Sect.3.2.) and then go on to show the individual potentials utilized to describe the various facets of material behavior (Sect.3.3.1.-3.3.5.), as well as exploring incremental updates (Sect.3.3.6.), all leading to the construction of the final incremental pseudo-potential (Sect.3.3.7.). The presentations of optimality conditions of the incremental pseudo-potential (Sect.3.4.) and of the stress update formulae (Sect.3.5.) conclude the description of the model. Applications of the model to two materials described in Stainier and Ortiz (2008) in Sect.4. aim to show some of its capabilities in describing coupled thermo-mechanical behavior.

## 2. INCREMENTAL FORMULATIONS FOR PURELY MECHANICAL PROBLEMS

In searching for variational formulations for general inelastic problems, the existence of a pseudo-potential function  $\psi$ , dependent on strains and internal variables describing the dissipative behavior of the material, is assumed. It is referred to as a pseudo-potential because, despite not being able to describe the state of stress for any strain state (i.e. despite not being hyperelastic in strict sense), it holds hyperelastic-like properties within the load increment:

$$\mathbf{P}_{n+1} = \frac{\partial \Psi(\mathbf{F}_{n+1}; \varepsilon_n)}{\partial \mathbf{F}_{n+1}} = 2\mathbf{F}_{n+1} \frac{\partial \Psi(\mathbf{C}_{n+1}; \varepsilon_n)}{\partial \mathbf{C}_{n+1}} \quad (1)$$

Where:  $\mathbf{P}_{n+1}$  is the first Piola-Kirchhoff stress tensor at load step  $n+1$ ;  $\mathbf{F}$  is the deformation gradient;  $\mathbf{C}$  is the right Cauchy-Green tensor; and  $\varepsilon_n$  is a set of internal variables, defined accordingly to the considered problem.

Such a formulation, based on the construction of an incremental pseudo-potential for every load step, is elsewhere explored in detail, e.g. in the works of Ortiz and Stainier (1999), Radovitzky and Ortiz (1999), Fancello et al. (2006) and Fancello et al. (2008). When no thermal effects are considered, the pseudo-potential used to describe a wide variety of inelastic problems takes on the following form:

$$\Psi(\mathbf{F}_{n+1}, \varepsilon_n) = \min_{\varepsilon_{n+1}} \{W(\varepsilon_{n+1}) - W(\varepsilon_n) + \Delta t \bar{\Psi}(\dot{\varepsilon}_{n+1}; \varepsilon_n)\} \quad (2)$$

Where  $W$  denotes a Helmholtz free energy density;  $\bar{\Psi}$  denotes a dissipation potential;  $\varepsilon$  includes external variable  $\mathbf{F}$  (deformation gradient) and internal variables  $\mathbf{F}^i$  (inelastic part of deformation gradient) and  $\mathbf{Q}$  (describing remaining internal processes); and  $\dot{\varepsilon}$  denotes the rate equations for the set of variables  $\varepsilon$ .

Since we wish to extend the previous formulation to a thermo-mechanical context, it is necessary to define an appropriate set of internal variables, to redefine the Helmholtz free energy density and to explore the laws of thermodynamics in order to build an incrementally consistent pseudo-potential.

## 3. EXTENSION OF THE VARIATIONAL FORMULATION TO THERMO-MECHANICAL VISCOPLASTIC PROBLEMS

### 3.1. Definitions and hypotheses

Before we delve into the thermodynamical aspects of the present model, some basic hypotheses are presented.

The classical multiplicative decomposition of the deformation gradient in elastic ( $\mathbf{F}^e$ ) and plastic ( $\mathbf{F}^p$ ) parts is also used here:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (3)$$

It is assumed that all plastic deformations are isochoric. Therefore, we may consider the following multiplicative decomposition of the deformation gradient, in volumetric ( $\mathbf{F}^{vol}$ ) and isochoric ( $\hat{\mathbf{F}}$ ) parts, and the consequent useful definitions of an isochoric elastic right Cauchy-Green tensor ( $\hat{\mathbf{C}}^e$ ), and the related natural strain ( $\boldsymbol{\varepsilon}^e$ ), both decomposed in their respective spectral quantities:

$$\mathbf{F} = \mathbf{F}^{vol} \hat{\mathbf{F}} \quad (4)$$

$$J = \det \mathbf{F} \quad \hat{\mathbf{F}} = \frac{1}{J^{1/3}} \mathbf{F} \quad (5)$$

$$\hat{\mathbf{F}} = \hat{\mathbf{F}}^e \mathbf{F}^p \quad \det \mathbf{F}^p = 1 \quad (6)$$

$$\hat{\mathbf{C}}^e = \hat{\mathbf{F}}^{eT} \hat{\mathbf{F}}^e = \sum_{i=1}^3 c_i^e \mathbf{E}_i \quad \boldsymbol{\varepsilon}^e = \frac{1}{2} \ln \hat{\mathbf{C}}^e = \sum_{i=1}^3 \varepsilon_i^e \mathbf{E}_i \quad \varepsilon_i^e = \frac{1}{2} \ln c_i^e \quad (7)$$

Considering a von Mises type flow rule for the plastic part, the rate of plastic deformation ( $\mathbf{D}^p$ ) may be decomposed in terms of amplitude ( $\dot{q}$ ) and direction ( $\mathbf{M}$ ). Ortiz and Stainier (1999) show that combining this decomposition with logarithmic strains and quadratic hyperelastic (Hencky) potentials yields a complete separation of kinematic aspects (direction  $\mathbf{M}$ ) and constitutive aspects ( $\dot{q}$ ). Thus, expressions similar to those of infinitesimal plasticity can be obtained.

$$\mathbf{D}^P = \text{sym}(\mathbf{L}^P) = \dot{\mathbf{F}}^P \mathbf{F}^{P-1} \quad (8)$$

$$\mathbf{D}^P = \dot{q} \mathbf{M} \quad \dot{q} \in \mathbb{R}^+ \quad \mathbf{M} \in K_M = \left\{ \mathbf{N} \in \text{Sym}: \mathbf{N} \cdot \mathbf{N} = \frac{3}{2}; \mathbf{N} \cdot \mathbf{I} = 0 \right\} \quad (9)$$

If a spectral decomposition of  $\mathbf{D}^P$  is used, it is possible to extend the separation of kinematic and constitutive aspects to more general potentials:

$$\mathbf{D}^P = \dot{q} \sum_{i=1}^3 q_i \mathbf{M}_i \quad (10)$$

$$\dot{q} \in \mathbb{R}^+ \quad q_i \in K_Q = \left\{ p_i \in \mathbb{R}: \sum_{i=1}^3 p_i = 0; \sum_{i=1}^3 p_i^2 = \frac{3}{2} \right\} \quad (11)$$

$$\mathbf{M}_i \in K_M = \left\{ \mathbf{N}_i \in \text{Sym}: \mathbf{N}_i \cdot \mathbf{N}_i = 1; \mathbf{N}_i \cdot \mathbf{N}_j = 0, i \neq j \right\} \quad (12)$$

The set  $K_Q$  enforces the traceless properties of  $\mathbf{M}$ , necessary since the plastic flow has to be incompressible and is considered irrotational (hypothesis of zero plastic spin), while the set  $K_M$  enforces properties of eigenprojections. The relations above allow for a complete representation of the plastic deformation gradient in terms of  $\dot{q}$ ,  $q_i$  and  $\mathbf{M}_i$ .

### 3.2. Thermodynamic aspects

The inclusion of thermomechanical coupling within the present variational formalism was firstly stated in Yang *et al.* (2006). In this paper we combine that approach with spectral decomposition (Eqs. 10-12) in order to allow the use of general isotropic hyperelastic laws suitable e.g. to polymeric materials.

We begin by postulating the existence a Helmholtz free energy density ( $W$ ), dependent on a set of external (an imposed  $\mathbf{F}$ ) and internal variables (cumulated plastic strain on the load step  $\Delta q = \dot{q} \Delta t$ , plastification directions  $q_i$ , eigenprojections  $\mathbf{M}_i$ , and temperature  $T$ ). Derivatives of the Helmholtz free energy density with respect to independent variables give thermodynamic forces associated to them. The entropy density per unit of undeformed volume ( $\eta$ ) is the thermodynamic force associated to the temperature  $T$ , just as the first Piola-Kirchhoff stress tensor ( $\mathbf{P}$ ) is the thermodynamic force associated to the total strain.

$$\mathbf{P} = \frac{\partial W(\mathbf{F}, q, q_i, \mathbf{M}_i, T)}{\partial \mathbf{F}} \quad (13)$$

$$\rho_0 \eta = - \frac{\partial W(\mathbf{F}, q, q_i, \mathbf{M}_i, T)}{\partial T} \quad (14)$$

By means of a Legendre-Fenchel transform of the equation above, we define the specific internal energy (per unit of undeformed volume) as:

$$U(\mathbf{F}, q, q_i, \mathbf{M}_i, \eta) = \sup_T [\rho_0 \eta T + W(\mathbf{F}, q, q_i, \mathbf{M}_i, T)] \quad (15)$$

We may now introduce the first law of thermodynamics in local form, as deduced by Holzapfel (2000), with  $\mathbf{H}$  denoting the heat flux vector,  $Q$  denoting local heat generation per unit undeformed volume and the term  $\mathbf{P} : \dot{\mathbf{F}}$  representing the stress power:

$$\dot{U} = \mathbf{P} : \dot{\mathbf{F}} - \text{Div} \mathbf{H} + Q \quad (16)$$

The second law of thermodynamics is then introduced, in a local form of the Clausius-Duhem inequality, where  $\dot{\eta}$  indicates the local production of entropy:

$$\mathbf{P} : \dot{\mathbf{F}} - \dot{U} + T \dot{\eta} - \frac{\mathbf{H}}{T} \cdot \text{Grad} T \geq 0 \quad (17)$$

The last term on the left-hand side indicates the production of entropy due to heat conduction. Heat flux occurs from warmer to colder regions of a body, which means that this term must be non-negative, i.e.:

$$-\frac{\mathbf{H}}{T} \text{Grad } T \geq 0 \quad (18)$$

A stronger form of the second law of thermodynamics, known as the Clausius-Planck inequality, introducing the concept of internal dissipation ( $\mathcal{D}_{\text{int}}$ ):

$$\mathcal{D}_{\text{int}} = \mathbf{P} : \dot{\mathbf{F}} - \dot{U} + T\dot{\eta} \geq 0 \quad (19)$$

Combining the Clausius-Planck inequality with the local form of the first law of thermodynamics presented above, we arrive at the energy balance in entropy form, which will later serve as the equation for entropy evolution along the load step of the incremental problem:

$$T\dot{\eta} = \mathcal{D}_{\text{int}} - \text{Div } \mathbf{H} + Q \quad (20)$$

In this paper, we consider an adiabatic case. No heat flux or heat generation are considered, so that the last two terms of the equation above are equal to zero. In other words, we consider thermal effects to be local, and temperature behaves as a local variable of similar nature to cumulated plastic strain  $\Delta q$ . All entropy production is due to internal dissipation during deformation, and is strictly associated to a dissipation potential that is a part of the incremental pseudo-potential, as shown below.

### 3.3. Incremental pseudo-potential

An additive decomposition of the free energy density is commonly used, representing the independence of elastic processes from internal processes, a very reasonable assumption for a wide range of materials. Furthermore, in the present work, we consider independent potentials for all different aspects of material behavior:  $\varphi^{\text{vol}}(J, T)$  is responsible for the elastic volumetric response;  $\varphi^e(\hat{\mathbf{C}}^e, T)$  represents the isochoric elastic response;  $\varphi^p(q, T)$  represents the plastic response of the material, including yield conditions and hardening; and  $\varphi^h(T)$  is responsible for the accumulation of energy in the form of heat.

$$W(\mathbf{F}, q, q_i, \mathbf{M}_i, T) = \varphi^{\text{vol}}(J, T) + \varphi^e(\hat{\mathbf{C}}^e, T) + \varphi^p(q, T) + \varphi^h(T) \quad (21)$$

It is important to observe that all the individual potentials are considered to be dependent of temperature. In other words, thermal effects affect potentials describing mechanical behavior, and are affected by them. The specific details of all individual potentials are presented below, followed by the description of the potential that describes dissipative behaviors of the material.

#### 3.3.1. Volumetric potential

The volumetric potential considers two distinct effects: the energy necessary to change the volume of a portion of material, proportional to the temperature dependent bulk modulus  $K(T)$ ; and the energy consumed in the thermal expansion of the material, proportional to the temperature change and the volumetric dilation coefficient  $\alpha$ .  $K_0$  is the bulk modulus at the reference temperature  $T_0$ .

$$\varphi^{\text{vol}}(J, T) = \frac{1}{2} K(T) (\ln(J))^2 - 3K_0 \alpha (T - T_0) \ln(J) \quad (22)$$

The temperature dependence of the bulk modulus, according to Holzapfel (2000), takes on the following linear form, where  $T$  is the current temperature:

$$K(T) = K_0 \left( \frac{T}{T_0} \right) \quad (23)$$

#### 3.3.2. Elastic isochoric potential

A Hencky potential, quadratic with respect to the logarithmic strain tensor, is used to describe the isochoric elastic response of the material. The elastic modulus  $\mu(T)$  elastic modulus, also according to Holzapfel (2000), follows a linear form with respect to the current temperature:

$$\varphi^e = \mu(T) \sum_{j=1}^3 (\varepsilon_j^e)^2 \quad (24)$$

$$\mu(T) = \mu_0 \left( \frac{T}{T_0} \right) \quad (25)$$

### 3.3.3. Plastic potential

The plastic potential was generalized from the model used in Vassoler (2007). It was chosen for its versatility in describing various types of plasticity, from purely elastoplastic to more complex higher order potential hardening models. Temperature dependence is introduced on coefficients  $\Sigma_0$ ,  $H$ ,  $\mu^p$  and  $\mu_j^p$ , in linear form similar to those presented previously. The exception is  $\Sigma_0$ , that decreases linearly with temperature increase, representing thermal softening of the yield criteria. Parameters  $\alpha^p$  and  $\alpha_j^p$  are considered temperature independent, as in equivalent parameters in Stainier and Ortiz (2008). The parameter  $q$  represents the cumulated plastic strain:

$$\varphi^p(q, T) = \Sigma_0(T)q + \frac{1}{2}H(T)q^2 + \mu^p(T) \left[ q + \frac{1}{\alpha^p} \exp(-\alpha^p q) \right] + \sum_{j=1}^N \frac{\mu_j^p(T)}{\alpha_j^p + 1} (q)^{\alpha_j^p + 1} \quad (26)$$

### 3.3.4. Potential of thermal energy accumulation

Associated to the specific heat capacity  $C_0$ , the potential of thermal energy accumulation accounts for portion of heat necessary to change the temperature of the material:

$$\varphi^h = \rho_0 C_0 \left[ (T - T_0) - T \log \frac{T}{T_0} \right] \quad (27)$$

### 3.3.5. Dissipation pseudo-potential

Dissipative behaviors are associated to the rate of the internal variables. For a viscoplastic models the dissipation potential depends on the rate of plastic deformation ( $\dot{q}$ ), usually represented by the rate of the cumulated plastic strain in the load step ( $\Delta \dot{q}$ ). Since the temperature is now an internal variable of the model, we would also need to include dependence on the rate of temperature change. We represent both rates together, following the work of Stainier (2006), by assuming that temperature and cumulated plastic strain appear together on all rate expressions. Thus, the following model, proposed by Stainier and Ortiz (2008), is adopted here to make use of the material parameters ( $m$ ,  $\hat{\varepsilon}_0$ ,  $b'$ ,  $d'$ ,  $n'$ ,  $\omega_1$ ,  $\hat{\omega}_1$ ,  $\omega_v$ ) and critical stresses ( $\sigma_1(T_0)$ ,  $\hat{\sigma}_1(T_0)$ ,  $\sigma_v(T_0)$ ) they already identified:

$$\bar{\Psi}(\dot{q}, q, T) = \sigma_y(q, T)\dot{q} + \frac{m}{m+1} \sigma_v(T) \hat{\varepsilon}_0 \left( \frac{\dot{q}}{\hat{\varepsilon}_0} \right)^{\frac{1}{m}+1} \quad (28)$$

$$\sigma_y(q, T) = \sigma_1(T)(1 + b'q)^{\frac{1}{n'}} + \hat{\sigma}_1(T)[1 - \exp(-d'q)] \quad (29)$$

$$\sigma_1(T) = \sigma_1(T_0)[1 - \omega_1(T - T_0)] \quad (30)$$

$$\hat{\sigma}_1(T) = \hat{\sigma}_1(T_0)[1 - \hat{\omega}_1(T - T_0)] \quad (31)$$

$$\sigma_v(T) = \sigma_v(T_0)[1 - \omega_v(T - T_0)] \quad (32)$$

Equation (34), the incremental counterpart of Eq. (28), is then stated by substituting rate quantities  $\dot{q}$  by  $\frac{T_{n+1} \Delta q}{T_n \Delta t}$ , which degenerates to the rate of cumulated plastic strain for  $\Delta t \rightarrow 0$  and  $T_{n+1} \rightarrow T_n$ , i.e., for sufficiently small load step. The cumulated plastic strain is substituted according Eq. (33), the incremental representation within the load step.

$$\Delta q = \dot{q} \Delta t = q_{n+1} - q_n \quad (33)$$

$$\bar{\Psi}(\Delta\dot{q}, \Delta q, T) = \sigma_v(q, T)\Delta\dot{q} + \frac{m}{m+1}\sigma_v(T)\dot{\varepsilon}_0 \left(\frac{\Delta\dot{q}}{\dot{\varepsilon}_0}\right)^{\frac{1}{m}+1} \quad (34)$$

The recourse to this strategy will show its importance during the minimization of the incremental pseudo-potential, described later.

### 3.3.6. Incremental updates

In an incremental context, it is necessary to determine evolution equations in terms of involved variables. An exponential mapping of the plastic part of the deformation gradient ( $\mathbf{F}^p$ ) is considered:

$$\mathbf{F}_{n+1}^p = \exp\left[\Delta q \sum_{i=1}^3 q_i \mathbf{M}_i\right] \mathbf{F}_n^p \quad (35)$$

The cumulated plastic strain for a certain point is considered to be the sum of the cumulated plastic strains of all previous steps:

$$q_{n+1} = q_n + \Delta t \dot{q} = q_n + \Delta q \quad (36)$$

This allows for us to substitute  $\dot{q}$  for  $\Delta q$  in the list of independent variables.

### 3.3.7. Incremental potential

We are now well equipped to assemble the incremental potential, consistently representing the material behavior within a load step. The total deformation gradient at the end of the load step ( $\mathbf{F}_{n+1}$ ) is imposed as an external variable. The fully coupled thermo-mechanical problem consists of solving the optimization problem (37) with respect to internal variables  $\Delta q$ ,  $\mathbf{M}$ ,  $q_i$  and  $T$  (grouped in the set  $\varepsilon$ ) indicated in the pseudo-potential  $\Psi(\mathbf{F}_{n+1}; \varepsilon_n)$ , thus completely determining the final state of the material. All quantities for load step  $n$  are considered known.

$$\Psi(\mathbf{F}_{n+1}, \varepsilon_n) = \inf_{\mathbf{M}_i, q_i, \Delta q, T_{n+1}} \sup \left\{ \Delta W(\mathbf{F}, \varepsilon) + \rho_0 \eta_n (T_{n+1} - T_n) + \Delta t \bar{\Psi} \left( \frac{T_{n+1} \Delta q}{T_n \Delta t}, T_n \right) \right\} \quad (37)$$

Where:

$$\Delta W(\mathbf{F}, \varepsilon) = W(\mathbf{F}_{n+1}, \varepsilon_{n+1}) - W(\mathbf{F}_n, \varepsilon_n) \quad (38)$$

Subjected to the following constraints:

$$q_i \in K_Q = \left\{ p_i \in \mathbb{R}: \sum_{i=1}^3 p_i = 0; \sum_{i=1}^3 p_i^2 = \frac{3}{2} \right\} \quad (39)$$

$$\mathbf{M}_i \in K_M = \{ \mathbf{N}_i \in \text{Sym}: \mathbf{N}_i \cdot \mathbf{N}_i = 1; \mathbf{N}_i \cdot \mathbf{N}_j = 0, i \neq j \} \quad (40)$$

$$\Delta q \geq 0 \quad (41)$$

### 3.4. Extremization of the pseudo-potential (inf-sup problem)

The minimization with respect to directions  $\mathbf{M}_i$  in Eq. (37) can be performed analytically. This step is omitted here due to space constraints, and is shown in detail in Fancello *et al.* (2008). It still remains an inf-sup problem with respect to  $(q_i, \Delta q)$  and  $T_{n+1}$  respectively that may be derived from the Lagrangian function:

$$\mathcal{L}(q_i, \Delta q, T_{n+1}) = \Delta W + \rho_0 \eta_n (T_{n+1} - T_n) + \Delta t \bar{\Psi} \left( \frac{T_{n+1} \Delta q}{T_n \Delta t}, T_n \right) + \lambda \left( \sum_{i=1}^3 q_i \right) + \beta \left( \sum_{i=1}^3 q_i^2 \right) \quad (42)$$

Considering a predictor state between configurations at time  $n$  and time  $n+1$ , consisting of a completely elastic step (the determination of directions  $q_i$  consist, then on determining the direction of radial return to the actual configuration),

we show the necessary optimality conditions for the problem next. Of note, is equation  $r_5$ , corresponding to the optimal condition with respect to current temperature  $T_{n+1}$ , that represents the local energy balance problem:

$$\varepsilon_i^e = \varepsilon_i^{e\text{pr}} - \Delta q \cdot q_i \quad (43)$$

$$r_i = \frac{\partial \mathcal{L}}{\partial q_i} = -\frac{\partial \Delta \varphi^e}{\partial \varepsilon_i^e} \Delta q + \lambda + 2\beta q_i = 0 \quad i = 1,2,3 \quad (44)$$

$$r_4 = \frac{\partial \mathcal{L}}{\partial \Delta q} = -\sum_{i=1}^3 \frac{\partial \Delta \varphi^e}{\partial \varepsilon_i^e} q_i + \frac{\partial \Delta \varphi^p}{\partial \Delta q} + \frac{T_{n+1}}{T_n} \frac{\partial \bar{\Psi}}{\partial \Delta q} = 0 \quad (45)$$

$$r_5 = \frac{\partial \mathcal{L}}{\partial T_{n+1}} = \left( \frac{\partial \Delta \varphi^e}{\partial T_{n+1}} + \frac{\partial \Delta \varphi^p}{\partial T_{n+1}} + \frac{\partial \Delta \varphi^h}{\partial T_{n+1}} + \frac{\partial U}{\partial T_{n+1}} \right) + \rho_0 \eta_n + \frac{\Delta q}{T_n} \frac{\partial \bar{\Psi}}{\partial \Delta q} = 0 \quad (46)$$

$$r_6 = \frac{\partial \mathcal{L}}{\partial \lambda} = \sum_{i=1}^3 q_i = 0 \quad (47)$$

$$r_7 = \frac{\partial \mathcal{L}}{\partial \beta} = \sum_{i=1}^3 q_i^2 - \frac{3}{2} = 0 \quad (48)$$

With further conditions:

$$\Delta q \geq 0 \quad (49)$$

$$r_9 = r_4 \Delta q = 0 \quad (50)$$

### 3.5. Stress update

By building the incremental pseudo-potential presented in section 3.3.6., consistently variational within a load step, we achieve our desired initial goal, which was to determine the final stress state of the material at time  $n+1$ , as in Eq.(1). Considering the separation between volumetric and isochoric parts, the expressions for the Piola-Kirchhoff ( $\mathbf{P}_{n+1}$ ) and Cauchy ( $\boldsymbol{\sigma}_{n+1}$ ) stresses are as follows:

$$\mathbf{P}_{n+1} = 2\mathbf{F}_{n+1} \frac{\partial \Psi(\mathbf{F}_{n+1}, \varepsilon)}{\partial \mathbf{C}_{n+1}} = \mathbf{F}_{n+1} \left[ J_{n+1}^{-2/3} \text{DEV} \left( 2 \frac{\partial \Delta \varphi^e}{\partial \hat{\mathbf{C}}_{n+1}} \right) + \frac{\partial \Delta \varphi^{\text{vol}}}{\partial J_{n+1}} J_{n+1} \mathbf{C}_{n+1}^{-1} \right] \quad (51)$$

$$\boldsymbol{\sigma}_{n+1} = \frac{1}{J_{n+1}} \mathbf{P}_{n+1} \mathbf{F}_{n+1}^T \quad (52)$$

## 4. APPLICATION TO SELECT MATERIALS

In order to show the capabilities of our model, we take advantage of the complete thermo-mechanical characterization of two metallic materials presented in the work of Stainier and Ortiz (2008): rate dependent  $\alpha$ -titanium alloy and pure polycrystalline tantalum. We basically seek to evidence thermo-mechanical coupling through stress-strain and temperature increase curves of numerically simulated uniaxial traction tests.

While the application of our model to  $\alpha$ -titanium is straightforward, characteristic temperature-dependent behavior of tantalum requires slight alterations. Considering previous works on tantalum, Stainier and Ortiz (2008) different temperature dependences in the potential for the dissipative behavior, considering thermally-activated processes (motion of dislocations through Peierls barriers) that result in the following expressions for critical stress  $\sigma_v(T)$  and material parameter  $\dot{\varepsilon}_0(T)$  (considered independent of temperature for  $\alpha$ -titanium):

$$\sigma_v(T) = \sigma_v(T_0) \frac{T}{T_0} \quad (53)$$

$$\dot{\epsilon}_0(T) = \dot{\epsilon}_0(T_0) \exp \left[ -T_c \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (54)$$

Material properties for both materials are presented on Table (1) below:

Table 1. Material properties for rate dependent  $\alpha$ -titanium alloy ( $T_0 = 293\text{K}$ ) and pure polycrystalline tantalum ( $T_0 = 298\text{K}$ )

Material property	Rate dependent $\alpha$ -titanium alloy ( $T_0 = 293\text{K}$ )	Pure polycrystalline tantalum ( $T_0 = 298\text{K}$ )	Material property	Rate dependent $\alpha$ -titanium alloy ( $T_0 = 293\text{K}$ )	Pure polycrystalline tantalum ( $T_0 = 298\text{K}$ )
$\mu(T_0)$ [MPa]	43,3	68,9	$\sigma_1(T_0)$ [MPa]	300,0	210,0
$K_0$ [GPa]	129,9	206,7	$\omega_1$ [ $\text{K}^{-1}$ ]	0,0008	0,0018
$\alpha$ [K]	$8,9 \cdot 10^{-6}$	$6,6 \cdot 10^{-6}$	$\hat{\sigma}_1(T_0)$ [MPa]	200,0	0,0
$\rho$ [ $\text{kg}/\text{m}^3$ ]	4500,0	16650,0	$\hat{\omega}_1$ [ $\text{K}^{-1}$ ]	0,0	-
$C_0$ [J/(kg.K)]	518,0	140,0	$\sigma_v(T_0)$ [MPa]	50,0	125,0
$\Sigma_0(T_0)$ [MPa]	75,0	10,0	$\omega_v$ [ $\text{K}^{-1}$ ]	0,0006	-
$H(T_0)$ [MPa]	0,0	0,0	$b^*$	5,0	1,25
$\mu^p(T_0)$ [MPa]	120,0	15,0	$n^*$	1,5	1,0
$\alpha^p$	10,0	80,0	$d^*$	7,0	-
$\mu_j^p(T_0)$ [MPa], $j=1,2,3$	0,0	0,0	$T_c$ [K]	-	4200,0
$\alpha_j^p$ , $j=1,2,3$	0,0	0,0			
$\dot{\epsilon}_0(T_0)$ [ $\text{s}^{-1}$ ]	1,0	0,1			
$m$	5,0	8,3			

For  $\alpha$ -titanium, two sets of tests are presented. First (Fig.1), the effect of strain rate is demonstrated. Increase of stress with increased strain rate is demonstrated, for strain rates varying between 0,001/s (which Stainier and Ortiz (2008) consider quasi-static) and 10000/s (dynamic range). Coupling of thermo-mechanical aspects lead to different temperature increase levels during deformation. Higher strain rates represent higher internal dissipation and result in larger increases in temperature.

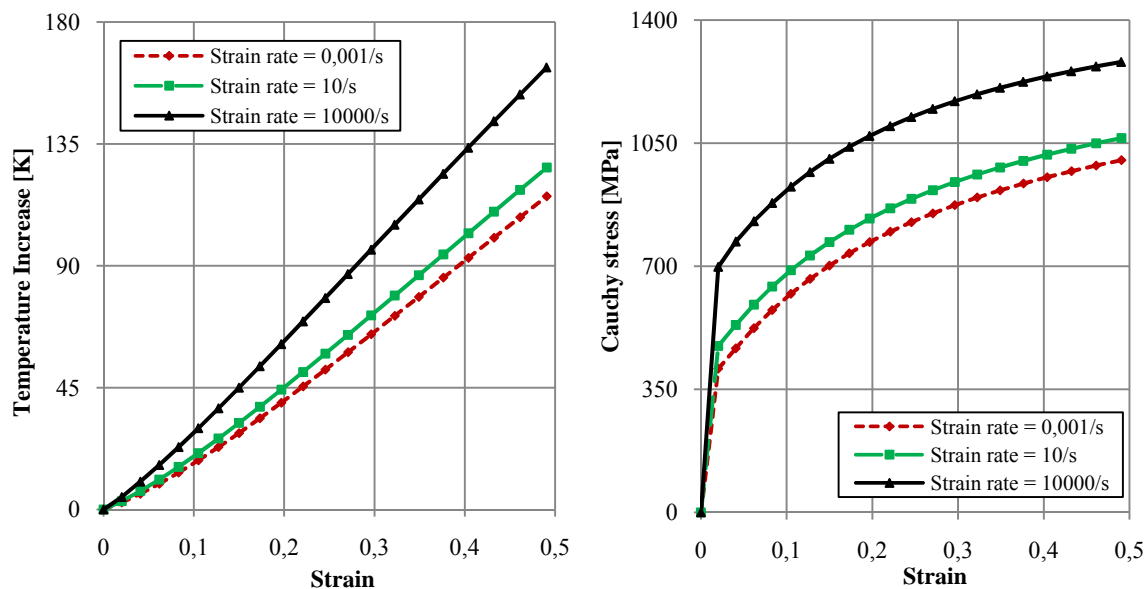


Figure 1. Influence of strain rate on temperature increase and stress-strain curves for rate-dependent  $\alpha$ -titanium alloy ( $T_0 = 293\text{K}$ )

A second set of tests (Fig.2) shows the influence of initial temperature on the thermo-mechanical behavior of the metal. Tests are simulated at a strain rate of 0,001/s. A higher initial temperature results in the need for lower stress levels in order to maintain the same strain rate level, i.e., thermal softening of  $\alpha$ -titanium is evidenced.



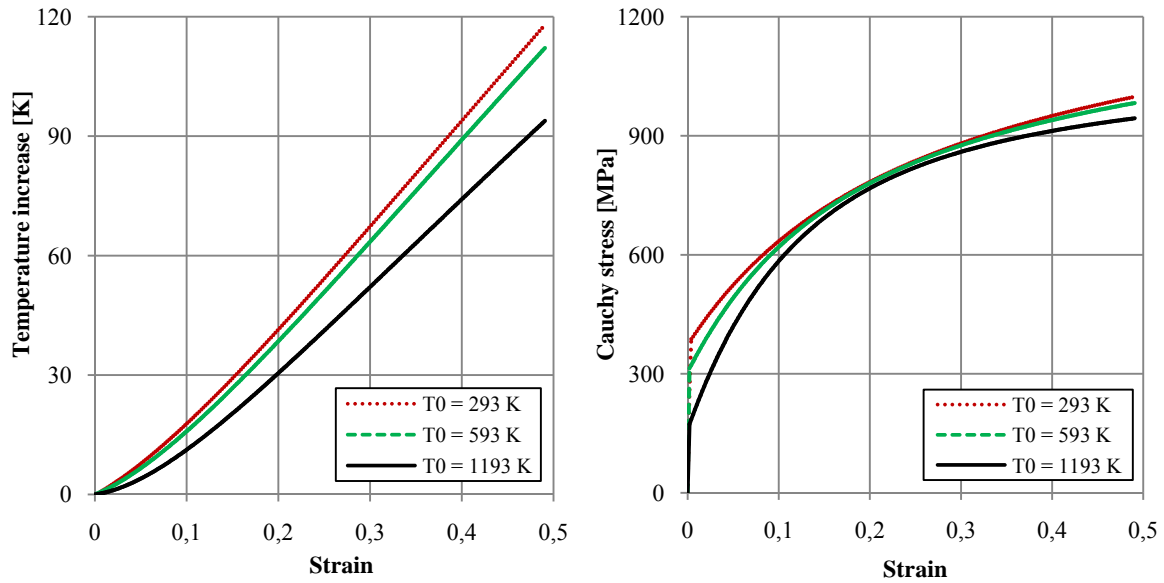


Figure 2. Influence of initial temperature on stress-strain and temperature increase curves for rate-dependent  $\alpha$ -titanium alloy (strain rate = 0,001/s).

Pure polycrystalline tantalum exhibits a very different behavior after plastification begins. The versatility of the model in describing a variety of materials is demonstrated in Fig.3, which shows the strain rate dependence of tantalum. Strain rates varying from 0,001/s to 10000/s are used, and the results in stress-strain behavior and temperature increase during deformation are shown.

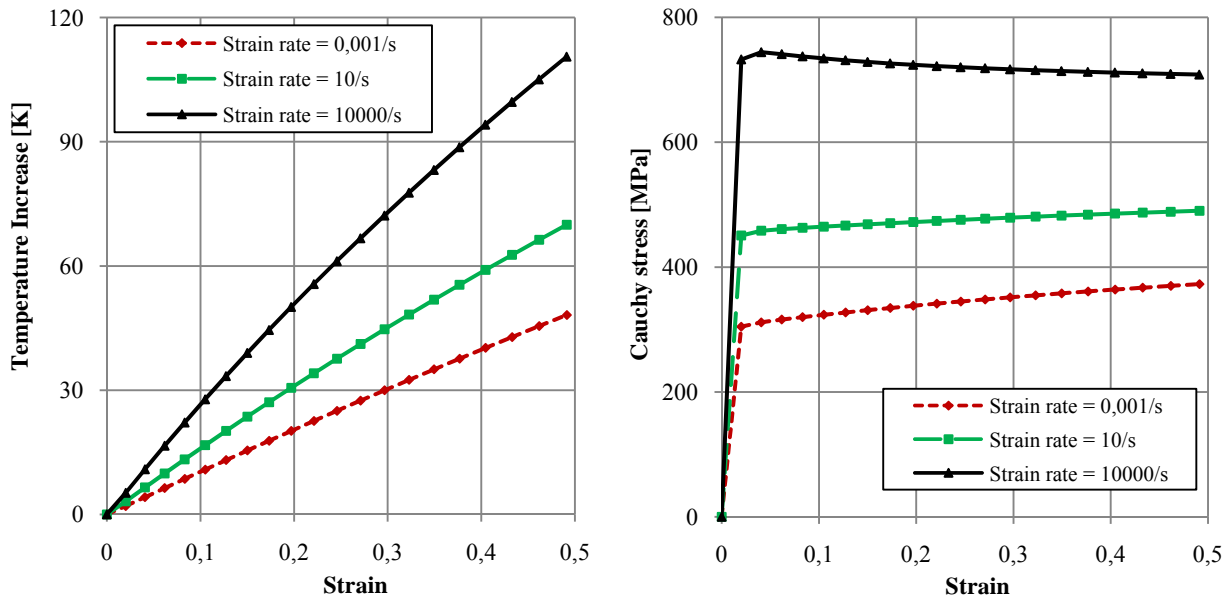


Figure 3. Influence of strain rate on stress-strain and temperature increase curves for polycrystalline Ta ( $T_0 = 298K$ ).

## 5. CONCLUSIONS

In this paper, we have shown the application of a variational formulation to a fully-coupled thermo-mechanical problem. Based on established models for a variety of inelastic material models, we defined appropriate potentials for the various aspects of material behavior involved in the finite thermo-viscoplastic problem. The general nature of the variational structure, with potentials dependent of spectral quantities, gives it great versatility in describing different sets of materials and material behaviors. The construction of an incrementally consistent pseudo-potential, together with the definition of constitutive updates for other variables, allows for the complete determination of the state of the material at

any point in time. As observed by Stainier and Ortiz (2008), the importance of having such a variational structure for the coupled thermo-mechanical problem, though not explored in the present paper, is ensuring the property of mathematical symmetry, which in turn brings about solid implementation advantages, such as symmetric tangent matrices.

The application of the model to two different metallic materials showed good correspondence to results found elsewhere in literature, both numerically simulated and experimentally observed. It was possible to estimate the increase in temperature during a uniaxial traction test, as well as to capture coupling effects in stress-strain curves with varying starting temperatures. Immediate applications of the model can include the *a posteriori* prediction of plastic work converted into heat, through the calculation Taylor-Quinney factor, as presented in Stainier and Ortiz (2008).

Limitations of the present model are associated to its simplifying hypotheses. As is, there is restriction to isotropic materials. No viscoelastic effects are considered, which may somehow limit its applications to some polymeric materials, though the extension to include such effects should pose no serious obstacles. It also important to highlight that this paper presented a model restricted to adiabatic thermo-viscoplasticity. Although the inclusion of heat conduction and heat generation is theoretically straightforward, their implementation is the subject of future works.

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