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Feature article

Thermo-mechanical modelling of rock-like materials at very high temperature: Application to ceramic refractories



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ABSTRACT

Rock-like materials like ceramic refractories, in working conditions may be subject to large temperature variations. To simulate practical applications, bespoke constitutive modelling is required. In this work a general, thermodynamically consistent framework, able to incorporate key micromechanical features of the material behaviour, and applicable to a wide range of geomaterials, is formulated and validated. Different thermodynamic potentials are proposed to deal with both reversibility and irreversibility. A key advantage of this approach is the ability to freely choose the thermal dependency interpolation functions. Extensive model validation is provided by correctly reproducing both reversible and irreversible experimental trends of different materials under different loading conditions. It is found that even for simple materials, if a sample is subject to a large stress level, its thermal and mechanical responses become unexpectedly coupled. The proposed modelling framework is not limited to refractories and can be easily adapted to different types of rock-like materials.

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1. Introduction

Several applications in manufacturing engineering imply the exposure of rock-like materials, like refractories, to very high temperature values, and possibly also large temperature gradients. Although several experimental programs have been carried out to measure relevant properties of ceramic refractories at high temperature, and some models (e.g., [1,17,25,27]) have been proposed to reproduce the main aspects of their thermo-mechanical behaviour, few attempts have been made to date to propose a general framework, able to incorporate key micromechanical features of the thermo-elasto-plastic material behaviour, with a thermodynamically consistent formulation, applicable to a wide range of different materials. Due to data availability, special focus in this work is given to ceramic materials used in the steel production industry. Based on their different behaviour upon thermal cycling, the two categories of (i) single component materials (like alumina) and (ii) casted or pressed composite refractories are identified, and their constitutive peculiarities are modelled with bespoke mechanisms.

Ceramic refractories are usually very stiff (with elastic stiffness ranging between 10 and 200 GPa) and characterised by thermal expansion coefficients usually ranging between $3 \times$ and

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 $6 \times 10^{-6} \text{ K}^{-1}$ (e.g., see [10,11,32]). When subjected to temperature variations of nearly 1500 K, the associated thermal strain is consequently very large (0.45-0.90%) which, if prevented, would lead to huge induced stresses (45-1800 MPa). Although refractory materials, to allow for their inevitable, thermally induced dilative deformation, are not usually constrained at the external boundaries, thermal gradients to which refractory pieces are subject in working conditions (e.g. in steel making processes) may be very large, thus possibly inducing large self-equilibrated internal stresses. Furthermore, certain refractory materials typically exhibit irreversibility upon temperature cycling, even at low applied stresses, which may lead to accumulated permanent changes (i.e. degradation) of their elastic and/or strength properties during their working life. Hence, simulating accurately the thermomechanical behaviour of these materials appears of paramount importance.

Thermo-mechanical and thermo-physical properties of refractories typically exhibit a wide variation among different materials, mainly depending upon their chemical composition, forming process and curing temperature. It has emerged from a comprehensive literature review [8] that while the specific heat capacity c_p (or c_v) and thermal expansion coefficient α exhibit characteristic trends of thermal variation that could be considered common to most ceramic material types, the modulus of elasticity *E* shows a much wider variety of trends with temperature. It appears that, somewhat counter to engineering intuition, the elastic modulus of certain refractories (both measured with dynamic techniques or

by means of mechanical, pseudo-static testing) does not exhibit a steady decrease with increasing temperature, but an initial horizontal or slightly decreasing trend, followed by a marked nonlinear increase, sometimes followed by an abrupt drop beyond a threshold temperature (e.g., see [10,16,17,32]). Moreover, while single component refractory materials exhibit a reversible thermal behaviour (thus if heated at very high temperatures and then cooled, they do not show any permanent change of their thermo-mechanical properties), composite materials exhibit hysteresis when subjected to a heating/cooling cycle (even at low applied stresses).

Overall, when measured in unconfined conditions, a general tendency is observed for both α and c_p to increase with increasing temperature, with a more or less marked tendency to reach a horizontal asymptote at large temperature values. This applies to both single-component materials such as alumina or glassy carbon (e.g. [32]) and composite materials, such as carbon-bonded refractories (e.g. [11]). In contrast, elastic stiffness exhibits a decreasing and mostly reversible trend with temperature for single component materials (e.g. [16]), while it shows the above mentioned nonlinear alternation of increasing and decreasing stages with increasing temperature, as well as some hysteresis upon temperature cycling, for composite (i.e., multi-component) materials (e.g. [17]). Similar trends have been experimentally observed also in the thermal evolution of material strength properties, such as the uniaxial tensile or compressive strength (e.g., [10,24]).

Due to the above mentioned heterogeneity of thermomechanical properties among different refractory materials, it is not possible to formulate a general constitutive model that can simulate properly all typical aspects of material response. Any thermo-mechanical constitutive model must be formulated and calibrated for the given composition and forming process that are peculiar of the specific material at hand, resulting in a somewhat restricted range of applicability.

In this work, some typical aspects of material response are considered, that apply to broad families of rock-like materials. Despite the main focus of this paper being on refractory materials, for which there is a certain availability of experimental measurements at high temperature, this work aims at proposing a general framework that could be easily applicable in an interdisciplinary context, to investigate the behaviour of geomaterials subjected to very high temperature. For example the same modelling approach can be applied to the natural counterparts of refractories, namely rocks, that in some contexts can be subjected to analogous thermomechanical loading conditions, such as those acting in shallow crustal phenomena (shear heating of faults and of rockslide slip planes [2,29]).

The limitations and implications of both basic and more complex constitutive assumptions concerning the thermo-elastic material response are discussed. In particular, the cases of reversible and irreversible thermo-mechanical behaviour upon thermal cycling at low applied stresses (i.e. within the elastic domain) are addressed. To capture irreversible response, a thermo-elastic model is also developed in the framework of elasto-plastic coupling (i.e., coupling between thermal, elastic and plastic properties is considered). A discussion follows on how the two thermo-mechanical elastic (reversible and irreversible) frameworks can be combined with a plastic driver to obtain a thermo-dynamically consistent, general elasto-plastic framework for refractory materials. Finally, the proposed framework is validated by reproducing numerically some experimentally observed trends.

Notation:

The following tensorial product will be used:

$$(\mathbf{A} \otimes \mathbf{B})[\mathbf{C}] = (\mathbf{B} \cdot \mathbf{C})\mathbf{A}$$
 and $(\mathbf{A} \underline{\tilde{\otimes}} \mathbf{B})[\mathbf{C}] = \frac{1}{2} (\mathbf{A}\mathbf{C}\mathbf{B}^T + \mathbf{A}\mathbf{C}^T\mathbf{B}^T)$,

for every second-order tensor **A**, **B** and **C**.

Basic assumptions:

The usual strain decomposition into the elastic and plastic strains will be assumed below, namely

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}_e + \boldsymbol{\epsilon}_p \quad \text{and} \quad \boldsymbol{\dot{\epsilon}} = \boldsymbol{\dot{\epsilon}}_e + \boldsymbol{\dot{\epsilon}}_p \tag{1}$$

where the dot stands for time derivative.

Moreover, following [27], the same decomposition is assumed to hold true for the entropy (per unit initial volume), namely

$$\eta = \eta_e + \eta_p$$
 and $\dot{\eta} = \dot{\eta}_e + \dot{\eta}_p$. (2)

Thus, absolute temperature θ plays the role of a stress-like quantity (cf. [27]), whereas the entropy plays the role of the corresponding (conjugated) strain-like quantity.

2. Thermodynamic potentials with reversible thermal behaviour

Let us first consider a refractory material undergoing negligible irreversible behaviour when subjected to a thermal loadingunloading cycle, under a small applied stress. The thermodynamic potential proposed in this Section assumes a perfectly reversible behaviour, thus the thermo-mechanical properties are assumed to remain unchanged after either a thermal, or mechanical, loadingunloading cycle, as long as the stress state remains within the yield surface.

Under non-isothermal conditions, the free energy per unit undeformed volume is expressed as

$$\psi = \psi(\boldsymbol{\epsilon}_{e}, \theta), \tag{3}$$

where ϵ_e is the small strain elasticity tensor and θ is the absolute temperature. Upon time differentiation, we obtain

$$\dot{\psi} = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}_e} \cdot \dot{\boldsymbol{\epsilon}}_e + \frac{\partial \psi}{\partial \theta} \dot{\theta}.$$
(4)

The definition of internal dissipation D_{int} involves the work done by the total stress with the corresponding work-conjugate strain rate, thus

$$\mathcal{D}_{\text{int}} = \theta \dot{\eta} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\epsilon}} - \dot{\boldsymbol{e}},\tag{5}$$

where σ is the stress tensor and e is the internal energy function $e = e(\epsilon_e, \eta_e)$, which is related to the free energy density through a Legendre transformation, as follows

$$\psi(\boldsymbol{\epsilon}_{e},\theta) = e(\boldsymbol{\epsilon}_{e},\eta_{e}) - \eta_{e}\theta.$$
(6)

In the case of purely thermoelastic response ($\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}_e$ and $\dot{\eta} = \dot{\eta}_e$), the insertion of Eq. (6) into Eq. (5) leads to

$$\mathcal{D}_{\text{int}} = \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\epsilon}}_e - \eta_e \theta - \psi \tag{7}$$

and the internal dissipation must vanish, $\mathcal{D}_{\rm int}=0,$ thus, through standard arguments [3], the following constitutive assumptions are obtained

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}_e}, \quad \eta_e = -\frac{\partial \psi}{\partial \theta}.$$
(8)

It should be noted that the above outlined approach, at variance with the thermoelastic theory proposed by Green and Naghdi [13] and further developed by [20], follows classic thermoelasticity, thus involving energy dissipation due to heat transfer. In the following, we analyse the implications of adopting the simplest possible class of ψ that can be deduced from published experimental results on refractory materials, namely

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