Computational Materials Science 116 (2016) 22–31

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

A multiphysics and multiscale approach for modeling microcracked thermo-elastic materials

Antonino Favata, Patrizia Trovalusci *, Renato Masiani

Department of Structural Engineering and Geotechnics, Sapienza University of Rome, Italy

ARTICLE INFO

Article history:
Received 4 July 2015
Received in revised form 30 September 2015
Accepted 25 October 2015
Available online 18 November 2015

Keywords:
Continua with microstructure
Heterogeneous materials
Non-classical thermal conduction
Microtemperature
Coarse-graining

ABSTRACT

In this contribution we propose a general framework able to describe the mechanical behavior of thermo-elastic materials with microcracks. The main features of our model come from the definition of additional kinetics descriptors, both mechanical and thermal. The model we propose is thermodynamically consistent and turns out to be non-local, in that it retains memory of the fine material structure through internal lengths and dispersion properties.

1. Introduction

The mechanical behavior of many materials of growing interest in materials science (such as composites, granular materials, alloys, liquid crystals) is often strongly influenced by an existing or emergent microstructure (such as microcracks, voids, defects, dislocations, phases in multiphase materials). Due to the different material properties of the microstructure, the macroscopic material turns out to be highly anisotropic and eventually inhomogeneous. Several approaches to the modeling of such materials can be found in the literature, and an account would necessarily be inappropriate in this context; for a synthetic description, the reader is referred to [70] and references therein. What is worth noticing is that, when a gross description is affordable – or the only possible to overcome an excessive computational effort – the description within the so-called *generalized continuum mechanics* is often indispensable, on extending the conventional mechanics in order to incorporate intrinsic microstructural effects in the mechanical behavior [23,45,13,22]. Our model falls within this framework, being considered as that of a *continuum with microstructure*, according to the definition of Capriz [13], namely a mathematical model of material bodies that retains memory of the microstructure, preserving the classical scheme of the continuum description. Each material point is identified by its position and a set of order parameters representing the inner structure; this scheme is compatible with the picture of a material point endowed with physical or geometrical properties, such as mass, porosity, extension, orientation and temperature field.

When, besides the purely mechanical behavior, one is interested to model the thermal effects of materials with microstructure, it is necessary to consider a generalization and/or a review of the classical theory adopted for simple continua, in order to capture the influence of the microstructure in thermal conduction; customarily, such a generalization is achieved by extending the state of variables by independent variables, as microrotation in Cosserat media and non-local heat flux [66,40,39].

In this paper, we propose a continuum model endowed with a mechanical and thermal structure able to predict the macroscopic behavior of a material with distributed microcracks, even if what we propose can be applied in a broader setting. The aim is to study the thermomechanical behavior of a material with distribution of pores or microcracks (due to manufacturing defects or lack of cohesion). To fix ideas, we focus on porous metal-ceramic composites (MCC, CMC) such as tungsten or titanium/molybdenum carbides (WC/Co, TiC/Mo_2C), alumina/zirconia materials (Al_2O_3/ZrO_2). The continuum with a just mechanical structure has been proposed in [72,42,79,78] and applied for particle/fiber reinforced polymer/ceramic matrix and masonry. Here we extend the microstructure to the thermomechanical framework, stemming from the ideas exposed in [24], where a simple and paradigmatic example of continua with (micro-)structure is exposed within the beams theory framework.

* Corresponding author.
E-mail addresses: antonino.favata@uniroma1.it (A. Favata), patrizia.trovalusci@uniroma1.it (P. Trovalusci), renato.masiani@uniroma1.it (R. Masiani).

http://dx.doi.org/10.1016/j.commatsci.2015.10.033
0927-0256/

The effects of cracks on the thermal conductivity have been investigated on various materials such as fiber-reinforced composites [41], optical coatings [58], graphite materials [52], thermal barrier coatings [49,16,65], clay [19] and others. The results of these studies can be roughly summarized in the fact that the thermal conductivity of materials decreases when they are affected by microcracks, due to the very low thermal conductivity of air void induced by cracks. The evidence of the presence of microcracks inside different materials was given by means of micrograph [16], topological sensitivity [11,10] and was quantitatively characterized to interpret the results on thermal conductivity [65]. Even X-ray micro-tomography can be considered as a powerful tool to monitor the spatial distribution of microcracks in materials [67].

In order to model the heat conduction in such materials, numerical models are employed, with a considerable computational effort. The use of discretization methods, such as finite element method [56,63], finite volume method [9,47,46] have the major difficulty in mesh generation process when the domain contains a numerous cracks of randomly geometries. In [3] the multi-region boundary element method (MR-BEM) to modeling the steady-state heat conduction in a heterogeneous system constituted by several homogeneous piecewise functions is employed. However, only a single or a few cracks are treated and the crack intersection is not considered in this application field. In [83] a multi-region boundary element approach is employed to obtain a boundary singular integral equation governing the steady state thermal transfer within this medium.

A model within the framework of generalized continuum mechanics, as the one we propose, may be computationally efficient, provided that a proper physical meaning of the additional fields is proposed and a constitutive identification for the internal and the external actions is performed [74,64,69,4,27,51,5,2,77]. In the present model, on the purely mechanical side, in addition to the standard displacement field, we consider a kinematical microstructural field, representing the mean jump of the displacement field due to the presence of microcracks; on the thermal side, we not only consider the thermal displacement, a nonstandard thermal state variable firstly considered by Helmholtz, but we also introduce an additional microstructural kinetic variable, whose time derivative represents the mean jump of the temperature field due to the presence of microcracks, and that we can call microtemperature. In [54], it is shown that the virtual power format can be so generalized as to deduce the balance laws of three-dimensional thermomechanics. On the other side, in [70,77] it has been shown that the Principle of Virtual Powers (PVP) can be expedient to perform coarse-graining procedures in the framework of the homogenization techniques. These corpuscular-continuous approaches are based on the assumption that a selected microscopic level structure of matter can be described as discontinuous, and that the transition from the coarse scale is governed by an *a priori* map between the large set of degrees of freedom od discrete systems and the deformation fields of the continuum. We contend that blending together these approaches can serve in properly defining the relevant balance equations and performing the constitutive identification. In fact, a better understanding of the physics behind the model, can be gathered from a finer description, where not only the kinematics appear clearer, but also the constitutive identification for the macroscopic and microscopic field can be properly carried out. With this purpose, we firstly deduce a macroscopic model, and then adopt such a finer description to justify our choices and to show a suitable definition of the macroscopic quantities in terms of the microscopic ones.

To frame our model in the non-standard thermodynamic setting it is necessary to claim that the idea to use an additional thermal descriptor is not completely new. It is worth mentioning that a theory of thermodynamics of elastic bodies with microstructure whose microelements possess microtemperatures is discussed in [33], where the Clausius–Duhem inequality is modified in order to include microtemperatures, and the first-order moment of the energy equations are added to the usual balance laws of a continuum with microstructure. Moreover, microtemperatures have been considered in [85,84], where were treated as known functions of the temperature and temperature gradients, and no balance equations were given for their determination; an application of a two-temperatures model to rod theory has been proposed in [1]. A study of heat conduction in materials with inner structure has been presented in [81,82,34,36]. In [35] the balance laws of micromorphic continua established by Eringen [21] and the entropy balance postulated by Green and Naghdi [29] are used to obtain a new theory of heat for materials with inner structure. In [57] a model of the thermoelastic theory without energy dissipation for materials with affine microstructure has been proposed. A micromorphic-type hyper-temperature and micro-entropy has been considered in [26], where a double temperature model is adopted.

The procedure we propose can be connected to classical homogenization techniques; nevertheless an important difference has to be pointed out: when dealing with these techniques an effective stiffness of the material is obtained, depending on the properties and the distribution of the microcracks (see for instance [12,38,62,61,59]); analogous results can be obtained for the effective thermal conductivity [60]. In our approach, both the mechanical and thermal properties are unaltered, while self-actions (both mechanical and thermal) are added. The results of the two different approaches can be compared in terms of macroscopic displacement [71] and temperature.

The paper is organized as follows. In Section 2, by using an extended version of the PVP, we deduce the *momenta* and *entropies balances* of the multifield (in that additional fields are considered) and multiphysics (in that mechanical and thermal physics are accounted for) continuum aimed at modeling a microcracked material. In Section 3, by using the framework of rational continuum thermo-mechanics, we deduce the constitutive restrictions and propose a suitable form of the free energy, which is functional to obtain a system of PDEs in terms of the kinetic variables. In Section 3, we connect our model to a finer description of the physics, going toward a multiscale constitutive identification. Finally, in Section 4, we propose some numerical results, intended to illustrate some of the potentialities of the model.

Our notation is direct. We let the order of a tensorial quantity be indicated by the font we use: in particular, we denote fourth order tensors by double struck capitals; second-order tensors by bold-face Roman or Greek capitals; vectors by bold-face, low-case Roman letters; and scalar fields by light-face, low case Roman or Greek letters. By the symbol "$\cdot$" we denote the inner product of two tensorial quantities of the same order, while the symbol $\otimes$ signifies dyadic product: $\mathbf{a}\otimes\mathbf{b}$ is a second order tensor, while $\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c}\otimes\mathbf{d}$ is a fourth order tensor. The appropriate notion of an inner product allows us to define transposition tensors: e.g. $\mathbf{A}^T\cdot\mathbf{a}\otimes\mathbf{b}=\mathbf{A}\cdot\mathbf{b}\otimes\mathbf{a}$, for all vectors $\mathbf{a}$ and $\mathbf{b}$. With sym and skw we denote the operators that yield the symmetric and skew-symmetric part of a second order tensor, respectively. The symbols $\nabla(\cdot)$, div $(\cdot)$ $\Delta(\cdot)$ denote the gradient, the divergence and the Laplacian operators, respectively. For Ψ a tensorial quantity of whatever order, the symbol $\dot{\Psi}$ denotes the derivative with respect to time.

2. Balance equations

Let us consider a continuum body pointwise identified with a reference region $\mathcal{C}$ of the ordinary Euclidean space. We regard $\mathcal{C}$ as a *microcracked* body, platform for two mutually interacting processes: (i) mechanical strain and stress, (ii) temperature variation.