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A length-dependent model for the thermomechanical response of ceramics

Jean-Baptiste Bouquet, Julian J. Rimoli *

School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

A R T I C L E I N F O

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A B S T R A C T

We present a length-dependent model for the thermomechanical response of ceramics through a concurrent multiscale scheme that accounts for: (i) the locally varying values of the sub-grain thermal conductivity tensor due to the interaction of phonons with microstructural features such as grain boundaries, and (ii) a continuum model of thermal stresses that explicitly resolves the polycrystalline structure of the material. At the sub-grain level, we compute the values of the thermal conductivity tensor using the Boltzmann transport equation under the relaxation time approximation. At the continuum level, the polycrystalline structure of the specimen is resolved explicitly by a finite element mesh and the texture of the polycrystal is assumed to be given. At this level, we adopt a Fourier model of heat conduction which utilizes values of thermal conductivity obtained at the lower scale. The mechanical response of the grains is modeled as elastic and anisotropic. The capabilities of the model are demonstrated through a series of examples, which highlight the potential of our approach for designing materials with improved thermomechanical response.

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1. Introduction

Predictive modeling of material behavior is a problem that necessarily spans several scales: e.g., inter-atomic interactions dominate the elastic behavior of materials, point and line defects condition their inelastic response, and planar defects such as grain boundaries could introduce length-dependent macroscopic material properties. With novel manufacturing and material synthesis techniques allowing the manipulation of characteristic material length scales, e.g., grain size (Razavi Hesabi et al., 2009; Chen and Wang, 2000; Wang et al., 2006a,b) and grain size distribution (Obare et al., 2012; Watanabe et al., 2002; Kieback et al., 2003), the possibility of designing microstructures for a desired macroscopic performance is becoming closer to reality. In this context, mesoscale models become key to link the fundamental processes obtained from the lower scales with the continuum models needed by designers and engineers.

As the characteristic size of the microstructure is reduced, length-dependent effects start becoming more relevant. Up to date, these effects have been studied separately: e.g., many authors have focused on the impact of length scale on thermal properties of materials (Lee et al., 2011; Maldovan, 2011a, 2012a,b; Wang et al., 2011; Fayette et al., 2000; Li et al., 2003), while others have considered mechanical length-dependent effects (Wang et al., 1989; Becher et al., 1998; Armstrong, 1970; Wang et al., 2008; Trunec, 2008). Despite these significant advances, the state-of-the-art in modeling the combined

* Corresponding author.
E-mail address: rimoli@gatech.edu (J.J. Rimoli).

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thermomechanical response of materials at the mesoscale still lags behind its counterparts at the atomic and continuum scales.

The main limitation of current mesoscopic thermomechanical models is that they consider length-scale independent thermal transport properties, or the equivalent assumption that the entire domain transitions from one equilibrium state to another with uniform temperature fields (Ortiz and Molinari, 1988; Tvergaard and Hutchinson, 1988; Zavattieri et al., 2001; Chen et al., 2010; Huang et al., 2015). In reality, as the characteristic length scale of the material is reduced, e.g., due to the presence of microstructural interfaces, its effective thermal conductivity decreases drastically (McConnell and Goodson, 2005; Goodson and Flik, 1993; Zou and Balandin, 2001; Maldovan, 2011a). In materials where heat conduction is mediated mainly by phonons, e.g., ceramics, this reduction is primarily due to the shortening of the bulk phonon mean free path (McConnell and Goodson, 2005; Goodson and Flik, 1993; Tang et al., 2011; Wang et al., 2011) as a result of scattering at the interfaces (Ziman, 2001; Cahill et al., 2003).

Available approaches to address this issue have their own limitations: molecular dynamics models are computationally prohibitive for problems of practical size (Ju and Liang, 2012), while thermal models purely based on kinetic theory are faster but currently limited to problems with simple geometries (e.g., thin films: Maldovan, 2011a; Jeong et al., 2012, wires: Maldovan, 2012a; He and Galli, 2012, or mono-sized polycrystals: Maldovan, 2011b), and have not been linked to mechanical models. Consequently, the development of predictive mesoscale models for the combined thermomechanical response of materials has remained an elusive goal.

This work provides, for arbitrary microstructural configurations, a concurrent multiscale framework able to capture local variations on thermal conductivity at the sub-grain level, the resulting variations on the mesoscopic temperature fields, and the consequent impact on thermal stresses.

The rest of the paper is organized as follows. The details of our concurrent multiscale model are outlined in Section 2. In Section 3, we demonstrate the capabilities of our model through three representative examples: the calculation of both the in-plane and cross-plane thermal conductivities of thin films, the anisotropy generated by the shape of a mono-crystal, and the influence that a graded grain size distribution has on the resulting temperature field as well as on the generated thermal stresses. Finally, Section 4 collects concluding remarks and discussion.

2. Formulation of the model

Our proposed model consists of: (i) a sub-micron scale model for the thermal conductivity based on the Boltzmann transport equation under the relaxation time approximation as described in Section 2.1, (ii) a classic Fourier heat transport model at the mesoscale as introduced in Section 2.2, and (iii) a continuum model of thermomechanical deformation that explicitly resolves the microscopic geometric features of the material as depicted in Section 2.3. Section 2.4 details the integration of all components of the model.

2.1. Subgrain-level model for thermal conductivity

Our subgrain-level model requires to accurately express the bulk thermal conductivity, as described in Section 2.1.1. Then, in Section 2.1.2, we consider the aforementioned effect of the reduction of the phonon mean free path on the thermal conductivity.

2.1.1. Bulk thermal conductivity

In materials where heat transfer is dominated by phonon transport, the bulk thermal conductivity can be estimated from the kinetic theory using the Boltzmann transport equation under the relaxation time approximation. This approach represents a particle-like view of heat transfer and accounts for both diffuse and ballistic transport effects. The bulk thermal conductivity D is calculated using the formula (Ziman, 2001; Kittel and McEuen, 1976)

$$D = \frac{k_b}{(2\Pi)^3} \sum_{P=L,T} \int_{BZ} \tau(\vec{k}) v_g^2(\vec{k}) \cos^2\alpha \left(\frac{\hbar\omega(\vec{k})}{k_b T} \right)^2 \frac{\exp(\hbar\omega(\vec{k})/k_b T)}{[1 - \exp(\hbar\omega(\vec{k})/k_b T)]^2} \, d\vec{k} \quad (1)$$

where k_b and $\hbar$ are respectively the Boltzmann and the reduced Planck constants, P is the polarization of the phonons, τ is the effective relaxation time, ω is the phonon frequency, T is the temperature, v_g is the phonon group velocity and α is the angle between the thermal gradient and the wavevector $\vec{k}$. The variable of integration $d\vec{k}$ is the elementary volume in the k-space, expressed as $d\vec{k} = dk_x dk_y dk_z = k^2 \sin\theta \, dk \, d\theta \, d\phi$, and the integration is performed over the first Brillouin zone (BZ) of the lattice. While the expression of the thermal conductivity generally involves an integral over frequency (Zhang, 2007; Holland, 1963), Eq. (1) consists of an integral over the phonon wavevector $\vec{k}$ such that it accounts for the direction of the phonon group velocity. The evaluation of the thermal conductivity requires the knowledge of several phonon properties such as the number of modes and the group velocity v_g, which can be obtained from the dispersion relations of the material. As noted by Holland (1963), the prediction of the thermal conductivity in semiconductors must incorporate the contribution of both longitudinal and transverse acoustic phonons. Due to their slow group velocity, we adopt the common assumption

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