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Micro-to-macro transitions for continua with surface structure at the microscale

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ABSTRACT

A geometrically non-linear framework for micro-to-macro transitions is developed that accounts for the effect of size at the microscopic scale. This is done by endowing the surfaces of the microscopic features with their own (energetic) structure using the theory of surface elasticity. Following a standard first-order ansatz on the microscopic motion in terms of the macroscopic deformation gradient, a Hill-type averaging condition is used to link the two scales. The surface elasticity theory introduces two additional microscopic length scales: the ratio of the bulk volume to the energetic surface area, and the ratio of the surface and bulk Helmholtz energies. The influence of these microscopic length scales is elucidated via a series of numerical examples performed using the finite element method.

1. Introduction

The effective macroscopic properties of a heterogeneous material can be estimated from the response of the underlying microstructure using homogenisation procedures. These mature procedures need to be extended in certain situations (e.g. when the microstructure contains nanoscale voids) to account for the role of the surface at the microscale. A surface typically exhibits properties different from those of the bulk. These differences, caused by processes such as surface oxidation, ageing, coating, atomic rearrangement and the termination of atomic bonds, are present in comparatively thin boundary layers. Surface effects are especially significant for nanostructures due to their large surface-area-to-volume ratio. The objective of this contribution is to present a novel micro-to-macro transition (computational homogenisation) procedure that accounts for the role of the surface at the microscale. Possible applications would be a bulk material with nanoparticles or a nanoporous structure.

The two main ingredients of the work presented here are (i) continuum formulations that account for surface effects and (ii) homogenisation as pioneered by Hill (1963). A brief review of these topics is now given.

1.1. State-of-the-art review of continuum formulations which account for surfaces

Two of the key approaches used to study the thermodynamics of surfaces and interfaces are:

- the zero-thickness layer or Gibbs (geometrical) method wherein a mathematical surface with zero thickness is introduced to capture excess quantities on the surface (see e.g. Gibbs, 1961);
- the finite-thickness layer method, which dates back to the work of van der Waals in the late 19th century, wherein a layer of finite thickness is employed in place of the interface.

The methodology adopted in this work is based upon the first approach. The reader is referred to Guggenheim (1940) for further details and a comparison of these two approaches.

Following the approach of Gibbs (1961), various models have been proposed to endow the surface or interface with their own distinct properties (see e.g Adam, 1941; Shuttleworth, 1950; Herring, 1951; Orowan, 1970). A widely-adopted continuum model, proposed by Gurtin and Murdoch (1975, 1978), gives the surface its own tensorial stress measures (see e.g Cammarata, 1994; Dingreville and Qu, 2005; He and Lilley, 2008; Duan et al., 2009, for applications in nanomaterials). It is the Gurtin and Murdoch model of surface elasticity that underpins the work presented in this contribution.

Park et al. (2006, 2007) and Park and Klein (2008) developed an alternative continuum framework based on the surface Cauchy–Born model, an extension of the classical Cauchy–Born model to include surface stresses.

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The thermodynamic fundamentals of surface science were reviewed in Rusanov (1996, 2005). Müller and Saul (2004) presented a review on the importance of stress and strain effects on surface physics. The role of stress at solid surfaces was critically examined by Ibach (1997). Fischer et al. (2008) studied the role of surface energy and surface stress in phase-transforming nanoparticles and reported on the thermodynamics of a moving surface.

The effect of surface energetics for ellipsoidal inclusions and the size-dependent elastic state of embedded inhomogeneities was investigated by Sharma et al. (2003), Sharma and Ganti (2004) and Sharma and Wheeler (2007). They utilised the classical formulation of Eshelby (1951, 1957) for embedded inclusions and modified it by incorporating surface energies. Duan et al. (2005a) extended the Eshelby formalism for inclusion/inhomogeneity problems to the nanoscale. Effective mechanical and thermal properties of heterogeneous materials containing nano-inhomogeneities based on the generalised Eshelby formalism are investigated in Duan et al. (2005a,b) and Duan and Karihaloo (2007), see also related works (Benveniste and Miloh, 2001, Huang and Sun, 2007, Fischer and Svoboda, 2010, Mogilevskaya et al., 2008, Lim et al., 2006, He and Li, 2006, Mi and Kouris, 2006, Yvonnet et al., 2011).

Our own contributions include the development in Javili and Steinmann (2009, 2010a) of a novel finite-element framework for continua with energetic surfaces. The framework inherently accounts for geometrical nonlinearities and surface anisotropy. The theory of thermoelasticity at the nanoscale is elaborated upon in Javili and Steinmann (2010b, 2011). A unifying review of various approaches for accounting for surface, interface and curve energies was presented in Javili et al. (2013).

A novel aspect of the work presented here is the development of a *geometrically non-linear* homogenisation framework accounting for surface energies at the microscale. To the best of the authors' knowledge, neither the theoretical nor the numerical aspects of the present problem have been studied previously.

1.2. State-of-the-art review of homogenisation

Homogenisation, as pioneered by Hill (1963, 1972), provides a consistent methodology to link the macroscopic and microscopic scales and forms the basis for computational micro-to-macro transitions (Suquet, 1987; Guedes and Kikuchi, 1990; Terada and Kikuchi, 1995; Smit et al., 1998; Miehe et al., 1999; Michel et al., 1999; Feyel and Chaboche, 2000; Kouznetsova et al., 2001; Miehe, 2002; Miehe and Koch, 2002; Temizer and Wriggers, 2008). Motivated by the non-classical behaviour of continua at the nanoscale, the objective of this contribution is to present a novel computational micro-to-macro transition framework for problems where the microstructure possesses surface structure. Within this framework, the response of the macroscopic problem is governed by the standard model of finite elasticity. The constitutive response of a macroscopic material point is obtained from the (numerical) solution of a representative problem at the microscopic scale. The microscopic problem contains surfaces possessing their own energetic structure.[2]

The contribution of the energetic surface to the overall strength of the microscopic representative volume element (RVE) depends on two relative microscopic length scales. The first is the ratio of the volume of the RVE to the area of the energetic surface. The second is the ratio of the microscopic Helmholtz energies of the surface and the bulk.

[2] The label energetic denotes that the surface possesses mechanical and constitutive structures. These structures are independent to those of the bulk. For an extensive discussion on the choice of material parameters used to describe the surface and their relation to those in the bulk, the reader is referred to Javili et al. (2012b) and the references therein.

The macro- and microscopic problems satisfy the assumption of scale separation. Nonetheless, the microscale problem possesses two relative length scales. Thus, unlike the case where the microstructure contains no energetic surfaces, the magnitude of the relative length scales of the microscopic problem are important. The energetic surface structure allows one to capture the phenomenon whereby the strength of a specimen increases with decreasing size. Standard micro-to-macro transition frameworks, i.e. where the macro- and microstructures possess no enhanced continuum description, can not capture this strengthening effect. This phenomenon has been investigated numerically using surface elasticity theory (see e.g. Wei et al., 2006; Kaptay, 2005; Javili and Steinmann, 2009, 2010a), but not within a micro-to-macro transition framework as is done in this contribution.

Various alternative approaches have been proposed to capture size effects within a micro-to-macro transition framework. In the spirit of their pioneering work on capturing size effects using gradient plasticity formulations (see e.g. Mülhaus and Aifantis, 1991; Zbib and Aifantis, 1989) Zhu et al. (1997) used a unit-cell technique to model size effects in metal matrix composites. Van der Sluis et al. (1999) proposed a methodology to couple a micromorphic macroscopic description (see e.g. Eringen, 1999, for an extensive overview of micromorphic media) to an underlying classical continuum in order to describe heterogeneous polymers. Kouznetsova et al. (2002) developed a micro-to-macro transition framework that allows information on the higher-order kinematic fields to be transferred to a microstructure described by a classical continuum formulation. Geers et al. (2007) and Coenen et al. (2010) investigated the response of macroscopic thin sheets with heterogeneous microstructure using second-order computational homogenisation schemes (Geers et al., 2001; Kouznetsova et al., 2002; Geers et al., 2003; Kouznetsova et al., 2004). The macroscopic response is described by a fourth-order shell theory. A second-order computational homogenisation scheme is then required to transfer the higher-order macroscopic kinematics to the microscopic problem. The opposite approach was adopted by Hirschberger et al. (2008) for material layers with a micromorphic mesostructure. Further important contributions on the interpretation of micromorphic material using homogenisation and the homogenisation of micromorphic microstructures have been made by Forest (1998, 1999) and Forest et al. (2001). McBride et al. (2012) developed a model for the computational homogenisation of energetic macroscopic layers containing underlying microstruture.

The influence of an interphase surrounding an inclusion was recently investigated by Li et al. (2011) using a closed-form approach based upon the model proposed by Mori and Tanaka (1973). The results were compared against finite element computations where the interphase was explicitly accounted for. The influences of size, interphase thickness, and inclusion shape were all accurately predicted. The surface elasticity theory adopted here can predict the same type of behaviour. In related work, Brisard et al. (2010) determined the Hashin–Shtrikman bounds on the shear modulus of a nanocomposite containing spherical inclusions and also accounted for the interface effects. Micro-to-macro transitions for coupled consolidation problems in micro-heterogeneous porous media have recently been considered by Su et al. (2011). Here the pore pressure at the microscale plays an important role.

1.3. Structure of the manuscript

This manuscript is organised as follows. The notation and certain key concepts are briefly introduced. The standard finite elasticity formulation governing the response of the macrostructure is summarised in Section 2. Thereafter the response of the microstructure containing an energetic surface is given. The link