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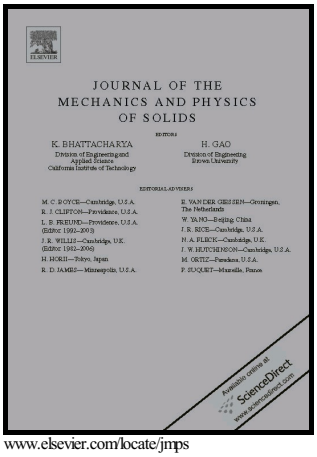

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PII: S0022-5096(16)30538-5
DOI: http://dx.doi.org/10.1016/j.jmps.2016.11.005
Reference: MPS3010

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 1 August 2016
Revised date: 2 November 2016
Accepted date: 4 November 2016

Cite this article as: Nikhil Chandra Admal, Jaime Marian and Giacomo Po, The atomistic representation of first strain-gradient elastic tensors, *Journal of the Mechanics and Physics of Solids,* http://dx.doi.org/10.1016/j.jmps.2016.11.005

The atomistic representation of first strain-gradient elastic tensors

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Abstract

We derive the atomistic representations of the elastic tensors appearing in the linearized theory of first strain-gradient elasticity for an arbitrary multi-lattice. In addition to the classical (2^{nd}-Piola) stress and elastic moduli tensors, these include the rank-three double-stress tensor, the rank-five tensor of mixed elastic moduli, and the rank-six tensor of strain-gradient elastic moduli. The atomistic representations are closed-form analytical expressions in terms of the first and second derivatives of the interatomic potential with respect to interatomic distances, and dyadic products of relative atomic positions. Moreover, all expressions are local, in the sense that they depend only on the atomic neighborhood of a lattice site. Our results emanate from the condition of energetic equivalence between continuum and atomistic representations of a crystal, when the kinematics of the latter is governed by the Cauchy-Born rule. Using the derived expressions, we prove that the odd-order tensors vanish if the lattice basis admits central-symmetry. The analytical expressions are implemented as a KIM compliant algorithm to compute the strain gradient elastic tensors for various materials. Numerical results are presented to compare representative interatomic potentials used in the literature for cubic crystals, including simple lattices (fcc Al and Cu, and bcc Fe and W), and multi-lattices (diamond-cubic Si). We observe that central potentials exhibit generalized Cauchy relations for the rank-six tensor of strain-gradient elastic moduli. In addition, this tensor is found to be indefinite for many potentials. We discuss the relationship between indefiniteness and material stability. Finally, the atomistic representations are specialized to central potentials in simple lattices. These expressions are used with analytical potentials to study the sensitivity of the elastic tensors to the choice of the cutoff radius.

Keywords: strain-gradient elasticity, materials length scales, Cauchy–Born rule, interatomic potentials

1. Introduction

The fundamental constitutive assumption of the classical continuum theory of elasticity is that the strain energy density of a solid depends on the first gradient of the deformation map (e.g. Malvern, 1977; Eringen, 1980; Truesdell and Noll, 2010; Marsden and Hughes, 1994). Such an assumption determines the structure of the boundary value problem of elasticity, and it gives rise to a theory without intrinsic length scales. As a consequence, classical elasticity theory fails to capture materials size effects and scaling of mechanical phenomena such as surface elasticity and dispersion of acoustic waves. Moreover, at the nano-scale, where the discrete atomic nature of matter becomes relevant, the theory predicts unphysical singularities in the elastic fields of crystal defects, such as cracks and dislocations.

Because of these intrinsic limitations of classical elasticity, during the last four decades atomistic methods have been developed to study nano- and micro-scale phenomena in materials mechanics. In the concurrent multiscale framework, methods were also developed to consistently bridge atomistic and continuum regions of a deformed body. For example, the *quasi-continuum* method developed by Tadmor et al. (1999) represents regions of high stress concentration (crack tips, dislocation cores, etc.), and surface defects where non-local effects dominate, using an atomistic model, while the rest of the body is described as a classical continuum. However, despite their potential, the spatial resolution of atomistic-continuum multiscale methods rapidly converges to that of direct atomistic models when dealing with heterogeneities such as surfaces or dislocations, which subjects them to limitations in the number of degrees of freedom they can handle. In addition, transport and time-dependent properties are exceedingly difficult to capture due to intrinsic heterogeneities in the atomistic/continuum coupling region, which results in reflections and unphysical phenomena.