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Surface effects in nanoscale structures investigated by a fully-nonlocal energy-based quasicontinuum method

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ABSTRACT

Surface effects in nanoscale mechanical systems such as nanoporous solids or small-scale structures can have a significant impact on the effective material response which deviates from the material behavior of bulk solids. Understanding such phenomena requires modeling techniques that locally retain atomistic information while transitioning to the relevant macroscopic length scales. We recently introduced a fully-nonlocal energy based quasicontinuum (QC) method equipped with new summation rules. This technique accurately bridges across scales from atomistics to the continuum through a thermodynamically-consistent coarse-graining scheme. Beyond minimizing energy approximation errors and spurious force artifacts, the new method also qualifies to describe free surfaces, which is reported here. Surfaces present a major challenge to coarse-grained atomistics, which has oftentimes been circumvented by costly ad hoc extensions of the traditional QC method. We show that our new coarse-graining scheme successfully and automatically reduces spurious force artifacts near free surfaces. After discussing the computational model, we demonstrate its benefits in the presence of free surfaces by several nanomechanical examples including surface energy calculations, elastic size effects in nano-rods and in plates with nano-sized holes. Overall, we demonstrate the importance of surface effects as well as a new strategy to accurately capture those computationally via coarse-grained atomistics.

1. Introduction

The mechanical behavior of nanoscale structures and nanostructured solids can deviate significantly from the material response observed in bulk solids. Example systems include micro- and nano-electro-mechanical devices and functional cellular solids with micro- and nano-sized morphological features, which promise tremendous technological and scientific potential. Nanoporous metals excel through unique physical, chemical, and mechanical characteristics (Biener et al., 2007), owing to the abundance of free surfaces. Depending on their degree of structural order, one distinguishes between nanoporous foams and structural materials (or, lattice materials). Both display high strength and stiffness and an extremely low mass density (as low as a few mg/cm^3). In addition, lattice materials offer unprecedented opportunities for bottom-up-engineered materials (Schaedler et al., 2011; Montemayor et al., 2014).

The extremely low spatial resolution of such systems is responsible for a variety of mechanical size effects. In particular, the abundance of free surfaces at the nanoscale alters the effective material behavior both within the reversible elastic regime and beyond. Surface relaxation alters the local atomic arrangement close to the surface, which in turn affects the atomic interactions and thus alters the effective elastic moduli. This size effect has been observed experimentally in single-crystalline nano-structures such as during elastic bending of nano-sized beams (Wong et al., 1997) or of carbon nanotubes (Poncharal et al., 1999), as well as during tension–compression testing

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of nanowires, see e.g. Chen et al. (2006), Agrawal et al. (2008), Asthana et al. (2011), Zhu et al. (2012) and Chen et al. (2013). Since surface relaxation is confined to a few atomic layers, the elastic size effects become noticeable only at small wire diameters on the order of a few nanometers, whereas the bulk response dominates at larger sizes.

Beyond the elastic limit, surfaces interact with lattice defects, e.g. by acting as dislocation and vacancy sinks and sources. Remarkable increases of the tensile strength of single-crystal metallic whiskers with decreasing whisker diameter were first reported in the pioneering work of Taylor (1924) and later confirmed by Brenner's studies (1956,1957). Their research demonstrated what is now well-known as a structure-induced size effect in metals. Since then, there has been compelling experimental evidence that the strength of nano-sized single crystals exhibits a power-law dependence on the feature size (Zhu et al., 2009). Recent tension–compression experiments on metallic micro- and nano-pillars impressively demonstrated this extrinsic size effect, cf. Greer et al. (2009), Burek and Greer (2010) and Kim et al. (2011). In particular, a variety of micro-deformation studies have revealed strong size effects in Cu single crystals (Dehm, 2009; Kiener et al., 2006, 2008; Kiener et al., 2009; Maass et al., 2008; Jennings et al., 2010). At such small scales, three mechanisms play an important role: small volumes reduce the number of defects in a statistical fashion, and surfaces interact with defects. The increase in strength has been explained by dislocation starvation (Greer et al., 2005; Shan et al., 2008; Greer and Nix, 2006), source exhaustion (Rao et al., 2008; Norfleet et al., 2008), source truncation (Parthasarathy et al., 2007; Rao et al., 2007), or weakest-link mechanisms (Norfleet et al., 2008); see Greer et al. (2011) for a review. In addition, surfaces alter the local stress state with important consequences for nano-scale structures, see e.g. Gill (2007), Pugno and Aifantis (2011), Miri et al. (2011) and Grekov and Yazovskaya (2013).

From the modeling perspective, the study of nano-sized structural members is challenging. On the one hand, they reside outside the realm of traditional molecular dynamics (MD); computational costs severely limit the domain size that can be modeled as well as the range of viable strain rates (Derlet et al., 2003). On the other hand, size effects in nanoscale structures as well as surface–defect interactions hardly admit the use of the continuum hypothesis which forms the basis of most engineering models. Nonlocal and size-aware continuum models have been proposed to capture individual size effects at the nanoscale, see e.g. Miller and Shenoy (2000) and Chen et al. (2006), yet they are commonly tailored for particular mechanisms and not universally applicable. Furthermore, the specific length scales involved in nanoscale structures oftentimes prohibit a separation of atomistic and structural scales. This calls for a powerful multiscale simulation methodology that bridges across scales and is capable of modeling nano- to micrometer-sized objects at the accuracy of the underlying atomistic ensemble.

Various methods have been developed to bridge the scales. On the one hand, hierarchical models are the method of choice when a clear separation of scales can be assumed so that homogenization techniques can extract the effective constitutive response from the atomistic scale and pass it to the structural level, see e.g. Shephard et al. (2004), Chung (2004), Park et al. (2005), Clayton and Chung (2006) and Liu et al. (2006). On the other hand, concurrent scale coupling methods integrate different constitutive descriptions into a single-scale model by spatially separating domains treated e.g. by first-principles, MD, discrete defect mechanics, and continuum theories. Prominent examples comprise coupled atomistic/discrete-dislocation models such as CADD (Curtin and Miller, 2003; Shilkrot et al., 2004; Nair et al., 2010) and AtoDis (Brinckmann et al., 2012), furthermore the bridging domain method (Belytschko and Xiao, 2003) as well as MADD (Abraham et al., 1998; Broughton et al., 1999) which couples several scales. In such methods, a key challenge is the passing of information across interfaces between different model domains. Coarse-graining techniques circumvent this difficulty by applying the same lower-scale constitutive description to the entire model by up-scaling in space and/or in time. Examples include Coarse-Grained MD (Rudd and Broughton, 2005a,b) and the quasicontinuum (QC) method (Tadmor et al., 1996). While spatial and temporal coarse-graining are equally important, we here focus on coarse-graining in space. Thereby, the number of degrees of freedom is reduced by introducing geometric constraints, thus making the lower-scale accuracy available for efficient large-scale simulations, see Tadmor et al. (1996), Suryanarayana (2011) and Iyer and Gavini (2011) for examples. Coarse-graining in time (to transition from femtoseconds to minutes) can be added to the techniques investigated here but is beyond the scope of this paper; see e.g. Voter (1997, 1998), Sorensen and Voter (2000), Voter et al. (2002), Kim et al. (2014) and Venturini et al. (2014). Also, we focus on the response of crystalline ensembles at zero temperature. Finite temperature extensions can be applied to the presented spatial coarse-graining techniques, see e.g. Shenoy et al. (1999b), Dupuy et al. (2005), Kulkarni et al. (2008), Marian et al. (2010), Ariza et al. (2012), Tadmor et al. (2013) and Venturini et al. (2014).

Here, we concentrate on one such coarse-graining methodology, viz. the QC method, which enables us to extend the accuracy of an atomistic constitutive description to large sample sizes via an efficient coarse-graining technique. The remainder of this paper is organized as follows. Section 2 reviews the concepts and governing equations of the QC method, explains the new extensions of the model, and the particular challenges arising from free surfaces. Section 3 summarizes a series of numerical examples that demonstrate the benefits of the new method and the observed size effects, and Section 4 concludes our investigation.

2. The quasicontinuum method, summation rules, and free surfaces

2.1. The quasicontinuum method and its summation rules

The QC method (Tadmor et al., 1996) is a popular numerical scheme to bridge the scales in crystalline solids