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Thermo-coupled Surface Cauchy–Born theory: An engineering finite element approach to modeling of nanowire thermomechanical response

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ABSTRACT

There are remarkable studies geared towards developing thermomechanical analyses of nanowires based on quasiharmonic and Molecular Dynamics simulations. These methods exhibit limited applicability due to the associated computational cost. In this study an engineering finite-temperature model based on Surface Cauchy–Born theory is developed, where surface energy is accounted for in the prediction of the thermomechanical response. This is achieved by using a temperature-dependent interatomic potential in the standard Cauchy–Born theory with a surface energy contribution. Simultaneous calculation of thermal and mechanical stresses is achieved by eliminating the diagonalization matrix of entropy in the quasiharmonic system. This leads to a reduction in the degrees of freedom by more than 99% in comparison with equivalent Molecular Dynamics models. For the purpose of validation, results obtained on copper and nickel nanowires through the proposed method are compared with those of the more involved Molecular Dynamics simulations. This comparison verifies the significant reduction in the computational process with an acceptable accuracy. Hence, the proposed method provides a promising engineering tool without compromising the underlying physics of the problem and has potential implications in the effective modeling of the nanoscale thermomechanical behavior.

1. Introduction

Nanowires (NWs) have been under intense development in recent years due to their unique mechanical, optical and electrical properties. They are utilized in various applications including electronics (Sacchetto et al., 2009) and photonics (Yan et al., 2009). A further emerging field of their application is nanoelectromechanical systems (NEMS), where they are mainly utilized as transducers for high-resolution mass (Hanay et al., 2012) and force sensing (Sage et al., 2015). Measurements down to yoctogram (Chaste et al., 2012) and femtoNewton (Marago et al., 2008) are reported. Most of these techniques involve the dynamic-mode operation of the NW, where changes in the resonant behavior are monitored as indicators of external mechanical effects (Sadek et al., 2010; Gil-Santos et al., 2010; Yang et al., 2006). Hence, NWs serve as ultra-small mechanical components, where size reduction proves to be extra advantageous in sensing applications. The main advantages are associated with (i) their high frequencies of operation leading to high sensitivities and high resolution, (ii) their ability of deterministic integration with higher-order structures such as electrodes, and (iii) the ease of their use as transducers, especially through piezoresistivity in Si

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NWs (Walther et al., 2012; He and Yang, 2006; Sansa et al., 2014; Erdem Alaca, 2009), and stretchable conductors with metal NWs (Xu and Zhu, 2012; Yao and Zhu, 2015).

It is well known that mechanical properties exhibit a dramatic size dependence. For example, Cao and Chen (2008) reported a significant size dependence of the modulus of elasticity in ZnO NWs (Cao and Chen, 2008). Similarly, Cuenot et al. (2004). showed an increase in the modulus of elasticity in silver and lead NWs in smaller diameters (Cuenot et al., 2004). Further effects such as phase transformations in gold NWs (Diao et al., 2003) and pseudoelastic behavior in NWs made of shape memory alloys (Park et al., 2005) are linked to the reduction of size. As the mechanical behavior of NWs is core to the operation of the majority of NEMS applications, modeling of their mechanical properties becomes a critical task. It proves to be a challenging task as well, as size reduction leads to the dominance of quantum effects due to the confinement by free surfaces and interfaces (Wang and Herron, 1991). A key feature of a free surface or an interface is the difference in their atomic arrangement due to the lack of bonding neighbors. This leads to a different set of elastic properties of surfaces from that of the bulk, where fully coordinated atomic arrangements and balanced forces exist.

A wide range of analytical models for the size-dependent elastic properties at the nanoscale has recently been developed. These models are usually based on enhanced classical continuum mechanics that use a bulk/surface decomposition to study surface effects with varying nanostructure dimensions. For example, Wang and Feng (2009) and He and Lilley (2008) presented the surface effect on bending and resonance frequency of NWs by utilizing a surface layer of finite thickness and the Young–Laplace equation (Tadmor et al., 1996b). On the contrary, an extensive range of multiscale modeling studies investigates problems with continuum methods with an atomic-scale resolution. These techniques can generally be referred to as atomistic-based continuum analyses or quasicontinuum methods. In this approach a general continuum finite element formulation is utilized to characterize the mechanical response of a given system. A finite element analysis provides a continuum system with an adaptive model refinement to save fully atomistic details and supplies a multi-scale analysis capability by refining the mesh size near lattice defects and highly energetic regions such as stacking faults and dislocations (Tadmor et al., 1996b) and elastic and plastic deformations (Tadmor et al., 1996a) in solids. The main difference of the atomistic-based continuum analyses from classical finite element methods is the derivation of the constitutive response from an atomistic standpoint rather than empirical rules and phenomenological models (Tadmor et al., 1996b).

Recently, Park et al. (2006) proposed a multiscale Surface Cauchy–Born (SCB) method to capture atomic-scale surface stress effects based on decomposing the potential energy into bulk and surface components, where bulk and surface stresses constitute distinct terms in the variational equation. This decomposition is the basis of capturing surface energy as the size of the continuum body decreases and the surface energy becomes dominant (Park et al., 2006). This method was successfully utilized to demonstrate size dependence in the bending behavior (Yun and Park, 2009) and resonance frequency of metallic (Park and Klein, 2008) and Si (Park, 2008) NWs due to the free surface energy. Although the aforementioned atomistic-based continuum analyses can describe phenomena such as size-dependence, surface energy and crystal non-uniformity, their use is confined to cryogenic systems. As classical interatomic potentials such as Lennard-Jones (LJ), Embedded Atom Method (EAM) and Tersoff are defined in static atomistic systems at zero absolute temperature, modeling of the thermomechanical response in nanostructures with atomistic resolution constitutes a novel challenge in engineering applications.

Only recently the temperature-dependent interatomic potential was developed as an efficient molecular calculation technique to model high-temperature behavior (Subramaniyan and Sun, 2008). For example, in Molecular Dynamics (MD) simulations, the effect of temperature is accounted for by thermal vibrations of each atom, where the system is permitted to progress dynamically by integrating Newton's equations of motion for each atom over time for the atomic system. Dupuy et al. (2005) proposed a finite-temperature method by a combination of statistical mechanics and finite element calculations (Dupuy et al., 2005). Xiao and Yang (2006), Liu and Li (2007), Jiang et al. (2005) and Tang et al. (2006) developed a multiscale Helmholtz free energy method based on the Cauchy–Born approximation. In this method, the effect of the finite temperature is accounted for by the local harmonic approximation, which relates the entropy to the vibration frequencies of the system(Xiao and Yang, 2006; Liu and Li, 2007; Jiang et al., 2005; Tang et al., 2006).

The effect of free surface on mechanical properties is one of the most sought-after modeling aspects in NEMS. As NEMS designs and applications are under constant evolution, engineering approaches with straightforward, computationally less demanding numerical techniques relevant to operation conditions such as finite temperatures are highly needed. In this study, we present the Thermo-coupled Surface Cauchy–Born (TSCB) model, a continuum-based theory with multiscale coupling for the thermomechanical analysis of NWs at finite temperatures where surface stress has a significant contribution. Based on the developments of the MD and the Helmholtz free energy methods to capture surface effects at finite temperatures, the present work proposes to implement temperature in the definition of the interatomic potential as opposed to using temperature as a kinetic component in entropy calculations from quasiharmonic approximations. This is achieved by utilizing Engineering Molecular Mechanics (EMM) proposed by Subramaniyan and Sun (2008) as an alternative molecular simulation tool (Subramaniyan and Sun, 2008) within the SCB method. Compared to MD and quasiharmonic models the proposed method requires less computational power and provides a bridge between fundamental scientific modeling efforts and practical engineering applications without compromising accuracy.

In the remainder of this work the Surface Cauchy–Born hypothesis is introduced first, followed by the description of the combination of molecular mechanics with finite element calculations. The results of the finite element simulations are compared with traditional MD calculations for validation. The work is concluded by analyzing the accuracy of the proposed method for the prediction of the modulus of elasticity as an essential parameter in mechanical response