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A continuum model for the mechanical behavior of nanowires including surface and surface-induced initial stresses

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ABSTRACT

The continuum modeling of the mechanical behavior of nanowires has recently attracted much attention due to its simplicity and efficiency. However, there are still some critical issues to be solved. In this paper, we demonstrate the importance of accounting for the effects of initial stresses in the nanowires that are caused by deformation due to surface stresses; we note that such initial stresses have previously been neglected in most existing continuum models. By considering the local geometrical nonlinearity of strains during the incremental flexural motion, a new formulation of the Euler–Bernoulli beam model for nanowires is developed through the incremental deformation theory, in which effects of the surface stress, the surface-induced initial stress and surface elasticity are naturally incorporated. It is found through comparisons to existing experimental and computational results for both fcc metal and ceramic nanowires that the surface-induced initial stresses, which are neglected in the Young–Laplace model, can significantly influence the overall mechanical properties of nanowires. We additionally demonstrate and quantify the errors induced by using the Young–Laplace model due to its approximation of surface stresses acting on only the top and bottom surfaces of nanowires.

1. Introduction

Nanowires (NWs) have been intensely investigated due to their potential as the basic building blocks for nanoelectromechanical systems (Craighead, 2000; Feng et al., 2007). The significant surface effects on the mechanical behavior of NWs with increasing surface-to-volume ratio have been observed both theoretically and experimentally (Sharma et al., 2003; Mcdowell et al., 2008; Philippe et al., 2009). Various numerical approaches have also been developed to capture the distinct size dependence of NWs due to surface stresses including the molecular simulation (MS) (Park and Ji, 2006; Karpov et al., 2006; Agrawal et al., 2008; Zhang and Huang, 2009; Jiang and Batra, 2009; Park et al., 2009; Wang et al., 2010a) and various finite element-based approaches that account for surface effects in different ways (Park et al., 2006; Wei et al., 2006; Park and Klein, 2007; Yvonnet et al., 2008; Park and Klein, 2008; Yun and Park, 2009; He and Lilley, 2009; She and Wang, 2009; Javili and Steinmann, 2010).

For the sake of simplicity and efficiency, analytical continuum approaches are also highly attractive (Gurtin and Murdoch, 1978; Zhang et al., 2004; He et al., 2004; Lu et al., 2006; Huang, 2008; Bar On et al., 2010), and thus the bending and buckling behavior of NWs has been studied by using the classical beam theory integrated with (Gurtin and Murdoch's) linear surface elasticity theory (He and Lilley, 2008a,b; Wang and Feng, 2009). In these models, surface effects on the flexural deformation are considered by using the generalized Young–Laplace equation (Chen et al., 2006a), which results in an equivalent distributed loading term in the beam equation. However, there are still some open problems with respect to the success of such formulation. First, the Young–Laplace model (He and Lilley, 2008a,b) cannot correctly predict the bending behavior of NWs with different boundary conditions. For fixed/fixed NWs, good agreement between the model and experiments (Cuenot et al., 2004; Jing et al., 2006) is found for Pb and Ag NWs, respectively, where both predict a significant size-dependent stiffening of the Young's modulus (He and Lilley, 2008a). In contrast, significant discrepancy is observed for fixed/free NWs; specifically, the experiment by Zijlstra et al. (2008) found that the elastic moduli of free standing [100] Au nanorods agree well with the bulk values, but size variation of the effective Young's modulus is reflected by the Young–Laplace model (He and Lilley, 2008b). The Young–Laplace model also incorrectly predicts the recently experimentally observed size-dependent Young's modulus of silicon nitride nanocantilevers (Gavan et al., 2009). Specifically,

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