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Static, free vibration and stability analysis of three-dimensional nano-beams by atomistic refined models accounting for surface free energy effect

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ABSTRACT

This work presents several higher-order atomistic-refined models for the static, free vibration and stability analysis of three-dimensional nano-beams. Stemming from a one-dimensional approach and thanks to a compact notation for the a priori kinematic field approximation over the beam cross-section, the model derivation is made general regardless the approximation order. This latter is a free parameter of the formulation. Several higher-order beam theories can be obtained straightforwardly. Classical beam models, such as Euler–Bernoulli's and Timoshenko's, are obtained as particular cases. The assumed constitutive equations for orthotropic materials account for the surface free energy effect as well as the third-order elastic constants. The resulting stiffness coefficients depend upon the cross-section side length. The governing equations and boundary conditions are variationally obtained through the Principle of Virtual Displacements. A Navier-type, strong form solution is adopted. Simply supported beams are, therefore, investigated. Static, free vibration and buckling analyses are carried out in order to investigate the effect of the cross-section side as well as the crystallographic plane orientation on the mechanical response. Beams with different values of the length-to-thickness ratio are considered. Results are validated in terms of accuracy and computational costs towards three-dimensional FEM solutions. Numerical investigations show the advantages of refined beam models over the classical ones demonstrating that accurate results can be obtained with reduced computational costs.

1. Introduction

Nano-beams hold a promise for a wide variety of applications such as sensors, actuators, transistors, probes and resonators in nano-electro-mechanical systems and biotechnology. Due to their great technological interest and potential applications, many researchers devoted their effort toward the determination of the mechanical properties and mechanical response of nano-beams. It is well recognised that, for this type of structures the traditional continuum mechanics is no longer suitable. The reduced coordination of atoms near a free surface induces a corresponding redistribution of electronic charge that alters the binding situation, see Sander (2003). As a result, the energy of these atoms is, in general, different from that of the atoms in the bulk. The elastic moduli of the surface region, therefore, may differ from those of the bulk. When the size of the element is of the order of micrometers or higher, the surface region can be neglected since it is typically very thin (few atomic layers) and the overall modulus can be assumed as the bulk modulus of a structural element. In the size range of tens of nano-meters, where the surface-to-volume ratio is significant, the surface region can no longer be neglected in considering the overall elastic behaviour of nano-sized structural elements. The effective modulus of nano-sized structural elements should be rather considered and, by definition, it is size-dependent, see Dingreville et al. (2005). Nano-beam has always been considered as made of isotropic materials although Dingreville et al. (2005) showed that the effective modulus tensor is orthotropic. The third-order elastic constants of a perfect crystal lattice are also generally neglected. As far as the determination of the mechanical properties is concerned, Dingreville et al. (2005) developed a framework to incorporate the surface free energy (SFE) within the continuum mechanics. Analytical expressions were derived for the effective elastic modulus tensor of nano-sized structural elements accounting for both the effects of the SFE and the third-order elastic constants of the perfect crystal lattice. Explicit expressions of the effective elasticity tensors were obtained for thin films, wires and spherical particles. In the case of nano-wires and nano-films, the effective modulus tensor was found to be orthotropic. These effective elasticity tensors were derived in the framework of the classical continuum mechanics. They can be, therefore, used directly in continuum mechanics models for predicting the overall

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response of nano-sized structures. Dingreville and Qu (2007) developed a semi-analytic method to compute the surface elastic properties of crystalline materials. Using this method, surface elastic properties (such as the intrinsic surface energy density, intrinsic surface stress and surface elastic stiffness) are obtained analytically in terms of the inter-atomic potentials of the material. The equilibrium (or relaxed) position of the atoms near the free surface are required in these analytical expressions. The relaxed position of the atoms near the free surface can be obtained via a standard molecular simulation of a free surface, see, for instance, Dingreville and Qu (2007) and Dingreville (2007). This semi-analytical method reduces the amount of computation time significantly when compared with existing methods. It is worth pointing out that there are other techniques, such as the fluctuation methods, to calculate the elastic constants, see Zhen and Chu (2012) and Cui et al. (2007) and references therein. The fluctuation methods are generally used to calculate the elastic constants at finite temperature. The very recent deformation-fluctuation hybrid method proposed by Zhen and Chu (2012) is particularly useful for complicated many-body potentials for which the analytical second derivative of the energy is challenging or impractical to obtain. To the best of the authors' knowledge, nano-beams have been usually investigated through classical Euler–Bernoulli's (EBT) or Timoshenko's (TBT) beam models. Jiang and Yan (2010) investigated the SFE effect on the elastic flexural behaviour of nano-wires via Timoshenko's beam model, see Timoshenko (1921, 1922) and Timoshenko and Goodier (1970). Aydogdu (2009) presented a generalised non-local beam theory to study the bending, buckling and free vibration of nano-beams. Eringen's non-local constitutive equations were there used and, from a structural modelling point, classical as well as Reddy's and Levinson and Aydogdu theories were adopted. SFE influence on buckling and free vibration response of nano-beams was addressed by Fu et al. (2010). Wang and Feng (2009) studied the SFE effect on the stability of nano-wires under uni-axial compression. This paper presents a static, free vibrations and stability analysis of nano-beams investigating the influence on the mechanical response of the SFE and of the third-order material elastic constants. Several higher-order beam theories are derived by means of a unified formulation. This modelling framework has been previously derived for anisotropic plates and shells, see Carrera (2003), Carrera and Giunta (2009a,b) and Giunta et al. (2011b), and, recently, extended to macro-scale beam structures, see Carrera and Giunta (2010), Carrera et al. (2010, 2011), Giunta et al. (2011a,c, 2013) and Biscani et al. (2011). Through a concise notation for the displacement field, the governing differential equations and the corresponding boundary conditions are derived in terms of a "fundamental nucleo" that does not depend upon the approximation order. This latter can be assumed as a formulation free parameter. Displacement-based theories that account for non-classical effects, such as transverse shear and cross-section in- and out-of-plane warping, can be formulated. It is worth mentioning that no special warping functions need to be assumed. TBT and EBT classical models are obtained as particular cases. Slender and thick nano-beams are investigated. The proposed models are validated through comparison with three-dimensional FEM solutions showing that accurate results can be obtained with reduced computational costs.

2. Preliminaries

Beam structures are characterised by a dimension, the axial extension l, that is predominant when compared to the leading dimension of the cross-section Ω. This later is identified by intersecting the beam with planes orthogonal to its axis. Cross-section geometry and reference system are presented in Fig. 1. The displacement field is:

$$\mathbf{u}^T(x,y,z;t) = \{\, u_x(x,y,z;t) \quad u_y(x,y,z;t) \quad u_z(x,y,z;t) \,\} \tag{1}$$

u_x, u_y and u_z are the displacement components along x-, y- and z-axis, respectively. Superscript 'T' represents the transposition operator. Voigt's notation stress ($\boldsymbol{\sigma}$) and the linear strain ($\boldsymbol{\varepsilon}$) vectors are grouped into the following in- and out-of-plane components:

$$\boldsymbol{\sigma}_p = \begin{Bmatrix} \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \end{Bmatrix} \quad \boldsymbol{\sigma}_n = \begin{Bmatrix} \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{xz} \end{Bmatrix} \quad \boldsymbol{\varepsilon}_p = \begin{Bmatrix} \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \end{Bmatrix} \quad \boldsymbol{\varepsilon}_n = \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{xy} \\ \varepsilon_{xz} \end{Bmatrix} \tag{2}$$

The relation between the linear strain and displacement components are:

$$\boldsymbol{\varepsilon}_p = \begin{Bmatrix} u_{y,y} \\ u_{z,z} \\ u_{y,z} + u_{z,y} \end{Bmatrix} \quad \boldsymbol{\varepsilon}_n = \begin{Bmatrix} u_{x,x} \\ u_{x,y} + u_{y,x} \\ u_{x,z} + u_{z,x} \end{Bmatrix} \tag{3}$$

Eq. (3) can be written in a compact notation:

$$\begin{aligned} \boldsymbol{\varepsilon}_p &= \mathbf{D}_p \mathbf{u} \\ \boldsymbol{\varepsilon}_n &= \mathbf{D}_{np} \mathbf{u} + \mathbf{D}_{nx} \mathbf{u} \end{aligned} \tag{4}$$

$\mathbf{D}_p, \mathbf{D}_{np}$ and $\mathbf{D}_{nx}$ are the following matrices of differential operators:

$$\mathbf{D}_p = \begin{bmatrix} 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \end{bmatrix} \quad \mathbf{D}_{np} = \begin{bmatrix} 0 & 0 & 0 \\ \frac{\partial}{\partial y} & 0 & 0 \\ \frac{\partial}{\partial z} & 0 & 0 \end{bmatrix} \quad \mathbf{D}_{nx} = \mathbf{I}\frac{\partial}{\partial x} \tag{5}$$

where $\mathbf{I}$ is the unit matrix. Geometric non-linearities are considered for the axial strain component in a Green–Lagrange sense, see Reddy (2004):

$$\varepsilon_{xx}^{nl} = \frac{1}{2}\left(u_{x,x}^2 + u_{y,x}^2 + u_{z,x}^2\right) \tag{6}$$

Under the hypothesis of a linear elastic orthotropic material, the generalised Hooke law holds:

$$\boldsymbol{\sigma} = \hat{\mathbf{C}}\boldsymbol{\varepsilon} \tag{7}$$

$\hat{\mathbf{C}}$ is the effective material stiffness matrix. According to Eq. (2), the latter equation reads:

$$\begin{aligned} \boldsymbol{\sigma}_p &= \hat{\mathbf{C}}_{pp}\boldsymbol{\varepsilon}_p + \hat{\mathbf{C}}_{pn}\boldsymbol{\varepsilon}_n \\ \boldsymbol{\sigma}_n &= \hat{\mathbf{C}}_{np}\boldsymbol{\varepsilon}_p + \hat{\mathbf{C}}_{nn}\boldsymbol{\varepsilon}_n \end{aligned} \tag{8}$$

Matrices $\hat{\mathbf{C}}_{pp}, \hat{\mathbf{C}}_{pn}, \hat{\mathbf{C}}_{np}$ and $\hat{\mathbf{C}}_{nn}$ in Eq. (8) are:

$$\hat{\mathbf{C}}_{pp} = \begin{bmatrix} \hat{C}_{22} & \hat{C}_{23} & 0 \\ \hat{C}_{23} & \hat{C}_{33} & 0 \\ 0 & 0 & \hat{C}_{44} \end{bmatrix} \quad \hat{\mathbf{C}}_{pn} = \hat{\mathbf{C}}_{np}^T = \begin{bmatrix} \hat{C}_{12} & 0 & 0 \\ \hat{C}_{13} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \hat{\mathbf{C}}_{nn} = \begin{bmatrix} \hat{C}_{11} & 0 & 0 \\ 0 & \hat{C}_{66} & 0 \\ 0 & 0 & \hat{C}_{55} \end{bmatrix} \tag{9}$$

The effective material stiffness coefficients $\hat{C}_{ij}$ for nano-beams with square cross-sections accounting for surface free energy and the third-order elastic constants are obtained according to the method proposed by Dingreville et al. (2005). For the sake of completeness and clarity, the next section is devoted to this method as well as the salient aspects of the molecular mechanics simulation.

3. Effective elastic properties of square cross-section nano-beams with surface effect

A two-step approach for establishing a link between the atomistic structure of surfaces and the macroscopic bulk elastic material properties has been proposed by Dingreville et al. (2005). The surface free energy, that is a thermodynamic parameter of a continuum, is first formulated in a manner that accounts for the surface atomistic structure. This calculation is based on molecular dynamics. The resulting surface free energy is, then, used for the phenomenological description of the strain energy density for

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