JOURNAL OF NANOMATERIALS AND DEVICES
Oct-Dec 2023, VOL. 1, ISSUE 1, pp. 1-2
https://doi.org/10.61577/jnd.2023.100001

RESEAPRO JOURNALS

EDITORIAL

OPEN ACCESS

On the continuum modelling of nanostructures

Matteo Strozzi

Department of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, Reggio Emilia, Italy

ARTICLE HISTORY

Received 14 June 2023; Revised 4 September 2023; Accepted 10 September 2023

In recent years, nanotechnology has assumed an important role due to its extraordinary characteristics, already completely revealed or not yet fully studied. Researchers are continuously applying the basic ideas of nanotechnology in several fields, including medicine, biology and engineering, to improve the existing applications in a wide range of devices, ranging from transistors to micro-motors and to biological probes. However, conducting experimental and numerical studies at the nanoscale presents numerous challenges, including high economic costs associated with resonant spectroscopy and significant computational effort required for molecular dynamics simulations.

One possible way to reduce these difficulties is to employ classical continuum mechanics theories. However, these theories fail to accurately simulate the actual behavior of materials at the small scale. Indeed, the mechanical response of nano-structures is very different from the one of macro-structures due to dimensional effects, which do not manifest themselves at macro-structure level and are related to the inherent discrete nature of nanomaterials.

The first important dimensional effect at the nanoscale is surface stresses, see the fundamental studies of Gurtin and Murdoch [1,2]. In nanostructures presenting very high surface-to-volume ratio, the elastic behavior of the material on the external surface is different from the one of the materials within the mass of the structure due to elevated surface stresses. To incorporate the effect of the surface stresses into continuum mechanics equations, Gurtin and Murdoch proposed an advanced theory of elasticity known as the "theory of surface elasticity".

A second important dimensional effect at the nanoscale is strain gradients, as initially investigated by Mindlin RD [3,4]. Strain gradient theory affirms that materials should be modelled as collections of atoms, each one with its specific small-scale deformation mechanism, and therefore in the stress-strain relationships the related strain gradient terms must be added.

To this aim, in order to include the effect of the strain gradients vwithin the continuum mechanics equations, Mindlin developed a new theory of elasticity known as the "theory of elasticity gradient".

The third and last important dimensional effect at the nanoscale is nonlocal elasticity, see the relevant studies of A.C. Eringen [5,6]. In classical continuum mechanics models, the stress state at a specific point of a body depends on the strain state only at that point and not at the other points, thereby lacking dimensional dependence. However, at the nanoscale, the microstructure of the material, including the distances and configurations between atoms within the discrete lattice, becomes crucial. Therefore, the actual discrete structure of nanomaterials cannot be homogenized into a classical local elastic continuum, necessitating the adoption of Eringen's "theory of nonlocal elasticity".

Using classical continuum mechanics theories to model the mechanical behavior of nanostructures can give some additional problems beyond the previously described size effects.

For example, in the case of carbon nanotubes, their effective discrete structure can be modelled by means of a continuous thin cylindrical shell if equivalent parameters, i.e., Young's modulus, Poisson's ratio, and wall thickness, are properly considered. The choice of these equivalent parameters for the continuous modelling of the actual discrete nanostructures has been addressed in different ways in the literature. A reliable methodology appears to be the one adopted by Yakobson, who obtained the equivalent values of the flexural stiffness, tensile stiffness, and Poisson's ratio of the continuous shells comparing them with the values of strain energy obtained via molecular dynamics simulations [7]. Consequently, the equivalent values of Young's modulus and wall thickness were obtained by means of the equations of the tensile and flexural rigidity from the classical continuum elastic shell theory. It should be stressed that molecular dynamics simulations were adopted to investigate the deformation behavior in the study of Yakobson because this method can study and define the inherent properties of materials at a microstructural level that cannot be properly characterized by means of macroscopic experiments, like resonant Raman spectroscopy.

Another very relevant issue in the modelling of nanostructures is related to their intrinsic anisotropy. Actually, in order to properly simulate the mechanical behavior of nanomaterials, it is essential to set an anisotropic model able to describe the dependence of the main elastic properties on dimensions and configurations. For instance, Chang [8,9] proposed an anisotropic elastic shell model reporting the expressions of five peculiar elastic properties of single-walled carbon nanotubes, i.e., longitudinal Young's modulus and Poisson's ratio, circumferential Young's modulus and Poisson's ratio, and also longitudinal shear modulus, as a function of carbon nanotube radius and chirality indices, and showed the correctness of this anisotropic elastic model by means of comparisons with molecular dynamics simulations. In particular, he demonstrated that the relationship between Young's modulus and shear modulus of the isotropic elastic

***Correspondence:** Prof. Matteo Strozzi, Ph.D., Department of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, 42122 Reggio Emilia, Italy, e-mail: matteo.strozzi@unimore.it

continuum mechanics theory is not yet retained in the case of single-walled carbon nanotubes. It must be underlined that also the study of Chang is based on a molecular mechanics model, called the "stick-spiral model", in which the total potential energy of the nanostructure is a sum of different bond energy contributions: another time it is observed that molecular dynamics represents an essential tool to properly simulate the actual discrete behavior of the nanomaterials via continuous elastic models.

The last relevant issue is related to the computational effort in modelling the dynamic behavior of nanostructures. Nanomaterials possess extremely high natural frequencies (in the order of THz) and infinitesimal dimensions (in the order of nanometres). These properties, on one hand allow nanostructures to be properly adopted in advanced nano-electro-mechanical systems but, on the other hand, they can bring relevant numerical difficulties to the mathematical procedures if the governing equations are not nondimensionalized. Let us consider again carbon nanotubes: the displacement field can be nondimensionalized if divided by means of the carbon nanotube radius, and the time can be nondimensionalized by using a reference natural frequency, for example, the fundamental (lower) natural frequency of a circular ring under radial external force without circumferential inertia [10].

As a conclusion, to accurately study the vibrations of nanostructures, which exhibit extremely small dimensions and high natural frequencies, it is crucial to properly incorporate their inherent size effects into dimensionless constitutive equations that are the basis of innovative advanced anisotropic elastic models considering equivalent continuous geometric and material parameters.

Disclosure statement

No potential conflict of interest was reported by the author.

References

1. Gurtin ME, Ian Murdoch A. A continuum theory of elastic material surface. Arch Ration Mech Anal. 1975;57:291-323.
2. Gurtin ME. Murdoch AI. Surface stress in solids. Int J Solids Struct. 1978;14:431-440.
3. Mindlin RD. Microstructure in linear elasticity. Arch Ration Mech Anal. 1964;16:51-78.
4. Mindlin RD, Eshel N. On first strain-gradient theories in linear elasticity. Int J Solids Struct. 1968; 4(1):109-124.
5. Eringen AC. Linear theory of nonlocal elasticity and dispersion of plane waves. Int J Eng Sci. 1972; 10(5):425-435.
6. Eringen AC. On differential equations of nonlocal elasticity and solutions of screw dislocation and surface waves. J Appl Phys. 1983;54(9):4703-4710.
7. Yakobson BI, Brabec CJ, Bernholc J. Nanomechanics of carbon tubes: instabilities beyond linear response. Phys Rev Lett. 1996;76(14):2511-2514.
8. Chang T, Geng J, Guo X. Prediction of chirality-and size-dependent elastic properties of single-walled carbon nanotubes via a molecular mechanics model. Proc Math Phys Eng Sci. 2006;462(2072):2523-2540.
9. Chang T. A molecular based anisotropic shell model for single-walled carbon nanotubes. J Mech Phys Solids. 2010:58(9):1422-1433.
10. Soedel W. Vibrations of Shells and Plates (Third Edition). Marcel Dekker Inc., New York, 2005.

https://doi.org/10.61577/jnd.2023.100001