**EDITORIAL**

# Open Issues in Continuum Modelling of Carbon Nanotubes

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Carbon nanotubes (CNTs) were discovered in 1991 inside NEC Corporation laboratories by S. Iijima, who studied the synthesis of fullerenes and first prepared a new type of carbon structures, referred to as CNTs, which were described as "helical microtubules of graphitic carbon" [1].

Since CNTs have very high Young's modulus and tensile strength, together with very small diameter, then they can reach natural frequencies of the THz order and therefore can be used as high sensitivity resonators in many electro-mechanical devices such as sensors, charge detectors and oscillators.

In addition, the extremely high electric and thermal conductivity of CNTs, together with the very high transparency in the visible range, makes them promising candidates for innovative applications that include heat exchangers and energy conversion systems, with the role of advanced catalyst supports or electrodes in solar and fuel cells.

CNTs are divided in two main classes: single-walled carbon nanotubes (SWCNTs), given by graphene sheets rolled into cylinders, and multi-walled carbon nanotubes (MWCNTs), composed by concentric SWCNTs, where the different cylinders are connected by van der Waals interaction forces.

Due to their relevant applications in several mechanical components, vibrations of CNTs have been attracted much attention from researchers. Specifically, CNT vibrations have been studied by means of experimental, atomistic mechanics and continuum mechanics methods.

Resonant Raman spectroscopy (RRS) starts from the experimental measurement of CNT diameter by means of atomic force microscopy and investigates atomic structure, chirality and natural frequencies of CNTs. However, due to the high technological complexity and costs, experimental methods cannot be considered as efficient

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approaches to study mechanical behaviour of CNTs.

Molecular dynamics (MD) simulations consider CNT atoms as interacting point-like masses, where the vibrations of the free atoms are recorded for a certain time duration at fixed temperature. However, due to the high computational effort, atomistic mechanics methods cannot be easily applied to CNT structural simulation, specially MWCNTs, which incorporate a large number of carbon atoms.

Since theoretical models based on continuum mechanics are computationally more efficient than MD simulations and do not present the technological complexity and high costs of RRS, then continuous elastic models are the most commonly adopted methods for the study of CNT vibrations.

In these models, it is assumed that the effective discrete structure of CNTs can be replaced by means of an equivalent homogeneous elastic structure with a continuous distribution of mass and stiffness, not considering their intrinsic atomic nature and so reducing the number of degrees of freedom.

In order to carefully investigate the validity of continuum mechanics approaches for CNT vibrations, in the cases when the lattice structure of CNT is modelled with a continuous circular cylindrical shell, some very important open issues should be taken into account and properly discussed.

The first relevant issue to be taken into account in the modelling of CNTs as continuous elastic shells is given by anisotropy. CNTs are usually modelled as isotropic elastic shells; however, they present a chirality-induced anisotropic behaviour due to their discrete nature that cannot be captured by using an isotropic shell model.

To this aim, Chang et al. [2] developed a molecular mechanics model, called "stick-spiral model", able to correctly predict chirality and size-dependent elastic properties of CNTs. They found explicit expressions for longitudinal Young's modulus and Poisson's ratio, circumferential Young's modulus and Poisson's ratio, and longitudinal shear modulus in case of chiral SWCNTs. This molecular based anisotropic elastic shell model including chirality effects was validated via comparisons with RRS and MD data, proving that the classical relationship of isotropic elastic continuum mechanics between Young's and shear modulus is not valid for SWCNTs.

In addition to anisotropy, another relevant issue in the modelling of CNTs as continuous elastic shells is given by nonlocality. Classical continuum mechanics models assume that the stress state at a given point of the body is uniquely dependent on the strain state at that point, and they do not admit any intrinsic size dependence in the elastic constitutive equations; therefore, they are not able to identify the small-scale effect on CNT mechanical behaviour. On the other hand, Eringen's nonlocal elasticity theory assumes that the stress state at a given point of a body is a function of the strain field at every point of the body, where the scale effect is inserted in the constitutive equations as a constant nonlocal parameter.

Starting from Eringen's nonlocal elasticity theory, Fazelzadeh and Ghavanloo [3] developed a refined nonlocal anisotropic elastic shell model by calibrating the value of nonlocal parameter with the results of MD simulations to obtain the linear vibrations of CNTs with different chiralities, geometries and boundary conditions.

Besides anisotropy and nonlocality, in the specific case of MWCNTs a third relevant issue to be taken into consideration in the continuum modelling is given by van der Waals interactions between the concentric SWCNTs.

Ru [4] proposed a linear relationship between pressure due to van der Waals interaction and radial displacement for the buckling and vibration analysis of MWCNTs in which the interaction coefficient is constant, i.e., it is not dependent on the radius of the individual SWCNT. However, it is clear that this simplified formulation is not accurate in modelling van der Waals interactions.

In order to accurately describe van der Waals interaction forces in MWCNTs, He et al. [5] proposed a linear relationship between pressure due to van der Waals interaction and radial displacement where the interaction coefficient is radius-dependent. By using this refined formulation, natural frequencies of MWCNTs were analysed for different geometries and chiralities, obtaining an excellent agreement with MD results.

To conclude, as reported above, several advanced models have been proposed in the last decades for the continuum modelling of carbon nanotubes. However, it is important to develop new more accurate models, able to better capture the actual CNT behaviour derived by experiments and MD simulations. To this purpose, *Journal of Mechanical Materials and Mechanics Research*, a peer-review and open access journal, provides a good service platform for researchers to publish their works on advances in continuum modelling of carbon nanotubes.

## Conflict of Interest

There is no conflict of interest.

## References

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