Dynamic analysis of some noncarbon nanotubes using mixed atomistic-continuum model

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Abstract. The nonlinear dynamic response of some of the noncarbon nanotubes is investigated using mixed atomistic continuum modelling using newly calibrated Tersoff-Brenner type interatomic potential. The governing equations of motion for the dynamic system are derived from Hamilton's principle. The nonlinear discrete dynamic equations linearized using the Newton-Rapson method are solved in conjunction with Newmark's method. Finite element formulation in cylindrical coordinates is formulated using four nodded Kirchhoff-type field consistent elements to eliminate the membrane locking in the circumferential strain. The effect of different boundary conditions (BCs), forcing frequency, damping, and material nonlinearity on the transient response of different nanotubes is investigated in detail. The present results obtained from the mixed-atomistic continuum model are compared with those obtained from molecular dynamic (MD) simulation for the free vibration frequencies of noncarbon nanotubes.

Introduction

For the application of nanomaterials in nanoresonators, nanosensors, actuators, and transducers, the study of vibrational characteristics is one of the essential parameters. Vibrational characteristics of boron nitride nanotubes (BNNTs) are investigated using different methods such as the continuum mechanics approach [1], molecular dynamic (MD) simulation [2], and multiscale modelling [3]. The multiscale modelling approach is found to be computationally efficient with accuracy comparable to MD simulations. Motivated by our recent studies [4], on the transient response of noncarbon nanosheets and the potential application of these noncarbon nanomaterials (NCM) in the field of nano-electromechanical systems and other applications, we investigate the transient response of noncarbon nanotubes with point load ($Q = Q_0 \sin\omega_f \tau$). The nanotubes' dimensions are L = 9.8513 nm and R = 0.9984 nm respectively and the forcing frequency (ω_f) is taken equal to the fundamental frequency.

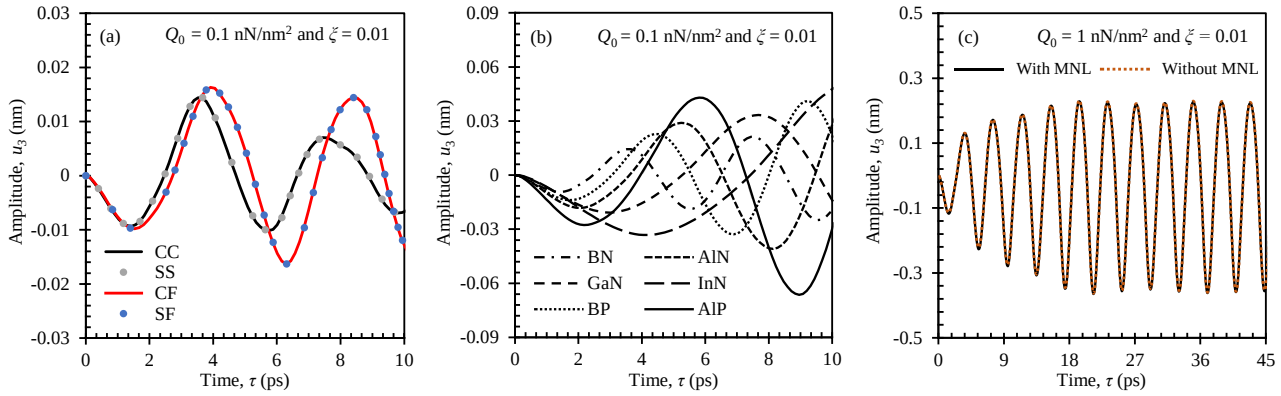

Figure 1: Transient response of (a) BNNT with different boundary conditions (b) different noncarbon nanotubes (c) BNNT with and without material nonlinearity (MNL).

Results and Discussion

It can be observed from Fig. 1(a) that the amplitude of vibration of BN is higher for clamped-free (CF) than clamped-clamped (CC). The amplitude of vibration for CC and SS (simply supported) is almost the same and the same is also found to be true for CF and SF boundary conditions. Among the different noncarbon nanotubes considered, AlP has the highest amplitude of vibration, and BN has the least amplitude under given loading this is because AlP has the least bending stiffness and BN has the highest bending stiffness (Fig 1(b)). From Fig. 1 (c) it can be observed that the effect of material nonlinearity on the transient response of nanotubes is insignificant.

References

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