MECHANICS OF DAMPING AND ENERGY DISSIPATION IN LOW-DIMENSIONAL GRAPHITIC NANOSTRUCTURES

Dong Qian*, Zhong Zhou*
*Mechanical Engineering, School of Dynamic Systems, University of Cincinnati, Cincinnati, OH 45221-0072, USA

Summary Low-dimensional graphitic nanostructures such as carbon nanotubes (CNTs) and graphene nanoplatelets (GNPs) have attracted significant attention for possible applications as reinforcement in nanocomposite, as sensors in nanoelectromechanical systems (NEMS), or as gigahertz oscillators in nanoscale device. Very limited work has contributed to research on damping properties and energy dissipation of CNT/GNP, which are important for a host of applications. Motivated by the significance of this important topic, we have developed a semi-analytical approach to understand the energy dissipation mechanism in CNTs and GNPs and their relation to damping and viscoelastic properties. A characteristic time scale is reported in the dynamic response of the CNTs and GNPs through relaxation. Energy dissipation peaks (or equivalently very low Q factors) have been reported in the range of Gigahertz excitations. The underlying mechanism for such trends is discussed in the context of thermoelastic theory.

INTRODUCTION

The rapid advances in nanofabrication and characterization have made possible the development of devices and materials with unprecedented strength, resolution, sensitivity and their applications. From the point of view of nanotechnological application of nanomaterial, energy loss or dissipation is generally universal in many devices and systems, and can not be simply neglected. One example is the development of nanoscale sensing resonators in which energy dissipation is directly related to sensitivity through Q factor. A semi-analytical approach is presented in this paper to study the damping mechanics with a focus on the intrinsic mechanisms in graphitic nanostructures such as carbon nanotubes (CNT) and graphene nanoplatelets (GNP). A theoretical model based on the theory of viscoelasticity is first established to predict the dynamic responses. Subsequently, the established model is verified through detailed atomistic model and simulation. With the verified model, an investigation on the various factors that contribute to the damping mechanisms is performed. We found interesting correlation between the Q factor and the load frequency. Dissipation peaks are revealed at certain critical load frequency.

APPROACH

Due to page limitation, we will outline our method in the context of multiwalled CNT beam oscillators. In this setting, we consider a MWCNT cantilever beam subjected to point load at the tip (See Figure 1 below).

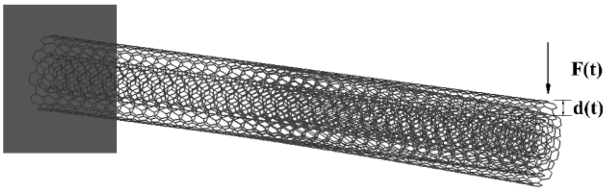

Figure 1: A MWCNT cantilever beam subjected to point load at the tip.

Based on the theory of elasticity, it can be shown that the F can be related to tip displacement through

$$d = \frac{FL^3}{3EI_{eff}} \tag{1}$$

where E is elastic modulus, L is the beam span and I_{eff} is an effective 2nd moment of area of the CNT beam cross section [1, 2]. By applying a hereditary integral operator [3-6] to linear elastic solution, we obtain the following time-dependent indentation displacement

$$d(t) = \frac{L^3}{6(1+\nu)I_{eff}} \int_{-\infty}^{t} J(t-\tau)\frac{dF(\tau)}{d\tau}d\tau \tag{2}$$

in which $J(t)$ is the creep compliance. We introduce the generalized Kelvin model [7] for the creep compliance

$$\boldsymbol{J(t)} = J_0 + \sum_{i=1}^{N} J_i(1-e^{-t/\tau_i}), \tag{3}$$

where $J_0 = J(0)$ is the instantaneous creep compliance representing the "instantaneous" elastic properties when the CNT/GNP is subjected to a dynamic load. The compliance coefficients $J_1, ..., J_N$ are discrete retardation spectra corresponding to the retardation times $\tau_1, ..., \tau_N$. If the time $t \gg \tau_i$, $J(t)$ converges to $J_\infty = \sum_{i=1}^{N} J_i$, which is referred to as the equilibrium creep compliance. The time variance is reflected in the Kelvin model and represents the so-called "delayed elasticity" since the equilibrium compliance is not achieved instantaneously. Subsequently, under a loading history $F(t)=v_0t$, a time-dependent load-displacement relationship is derived by combining Eqs.(1)-(3):

$$d(t)=\frac{L^3}{6(1+\nu)I_{eff}}\left\{\left(J_0+\sum_{i=1}^{N}J_i\right)F(t)-\sum_{i=1}^{N}J_iv_0\tau_i\left[1-\exp\left(-F(t)/(v_0\tau_i)\right)\right]\right\} \qquad (4)$$

To identify the creep compliance values and time constants in Eq.(4), molecular dynamics simulations will be performed to obtain the load-displacement relation and fitted to the model. Based on the generalized Kelvin model with a single retardation time, it can then be shown that the quality factor Q is given as

$$Q=\frac{J_0(1+4\pi^2\tau^2f^2)+J_1}{2\pi J_1\tau f}, \qquad (5)$$

where τ is the visco-elastic time constant, and f is the load frequency.

Table 1 lists the Q factors that are calculated for double-walled CNTs ((5,5) inside of (10,10)) under different load frequency and length to diameter ratio. The reduction of Q factor indicates enhanced energy dissipation at higher load frequency. In addition, higher L/D ratio yields lower Q factor values.

Table 1. Q factor of DWCNT (5,5)/(10,10) (D=1.356nm)

f (*GHz*)	3.18	6.37	9.55	12.74	15.92				
L/D	5	5	5	5	4	5	6	8	10
Q	666.7	322.6	277.8	222.2	256.4	166.7	125.0	42.5	21.7

CONCLUSIONS

We propose that the energy dissipation phenomenon reported here can be explained by the thermoelastic theory [8-10]. Based on this theory, energy is dissipated when heat flows irreversibly due to the temperature gradient. Such a gradient can be introduced due to the nonuniform strain field in the flexural deformation. If the time scale of the loading condition is compatible with the carrier of the heat, i.e., the phonons in this case, one would expect a close coupling between the deformation and temperature such that the energy dissipation is enhanced. The observed dependence of Q factor on the load frequency agrees well with the experiments. Details of comparison can be found in [6].

ACKNOWLEDGEMENTS

This work is supported by the National Science Foundation (Grants CMMI-0600583, 0700107 and 1120382). Any opinions, findings, conclusions, or recommendations expressed in these documents are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

References

[1] H. J. Qi, *et al.*, "Determination of Mechanical Properties of Carbon Nanotubes and Vertically Aligned Carbon Nanotube Forests Using Nanoindentation," *Journal Of The Mechanics And Physics Of Solids,* vol. 51, pp. 2213-2237, Nov-Dec 2003.

[2] A. Pantano, D. M. Parks, and M. C. Boyce, "Mechanics of Deformation of Single- and Multi-wall Carbon Nanotubes," *Journal Of The Mechanics And Physics Of Solids,* vol. 52, pp. 789-821, Apr 2004.

[3] E. H. Lee and J. R. M. Radok, "The Contact Problem for Viscoelastic Bodies," *Transactions of the ASME, Journal of Applied Mechanics,* vol. 27, pp. 438-444, 1960.

[4] Z. Zhou, D. Qian, and M.-F. Yu, "Energy Dissipation and Intrinsic Loss in Single Walled Carbon Nanotubes Due to Anelastic Relaxation," *Journal of Nanoscience and Nanotechnology,* vol. 11, pp. 1267-1272, 2011.

[5] Z. Zhou, D. Qian, and M.-F. Yu, "A Computational Study on the Transversal Visco-elastic Properties of Single Walled Carbon Nanotubes and Their Relation to the Damping Mechanism," *Journal Of Computational And Theoretical Nanoscience,* vol. 8, pp. 820-830, 2011.

[6] Z. Zhou, V. K. Vasudevan, and D. Qian, "Energy Loss in Carbon Nanotube Beam Oscillators due to Anelastic Relaxation," *Journal of Engineering Materials and Technology,* Accepted, 2011.

[7] R. M. Christensen, *Theory of viscoelasticity An introduction*. New York and London: Academic Press, INC., 1971.

[8] B. H. Houston, *et al.*, "Thermoelastic Loss in Microscale Oscillators," *Applied Physics Letters,* vol. 80, pp. 1300-1302, Feb 18 2002.

[9] C. Zener, "Internal friction in solids I. Theory and internal friction in Reeds," *Phys. Rev.,* vol. 52, p. 230, 1937.

[10] C. Zener, "Internal friction in solids II. General theory of thermoelastic internal friction," *Phys. Rev.,* vol. 53, p. 90, 1938.