Journal of
Computational and Theoretical Nanoscience
Vol. 8, 814–819, 2011

Boundary Condition and Strain Effects on the Quality Factors of Single Walled Carbon Nanotubes

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We utilize classical molecular dynamics to study energy dissipation (the Q-factors) of carbon nanotube-based nanoresonators undergoing flexural oscillations. Specifically, we have studied the difference in Q-factors of nanotubes with fixed/fixed and fixed/free boundary conditions. In doing so, we have found that fixed/fixed nanotubes have significantly higher Q-factors, particularly at low temperatures. Furthermore, we have found that mechanical strain can be utilized to enhance the Q-factors of fixed/fixed nanotubes by factors of 2–4 across a range of temperatures for tensile strains ranging from 0 to 6%. The results collectively indicate that fixed/fixed carbon nanotubes should be preferable for NEMS applications at low temperature due to a combination of inherently higher Q-factors, and the fact that the Q-factors can be further improved through the application of tensile strain.

Keywords: Nanotubes, Strain, Quality Factor, Boundary Conditions.

1. INTRODUCTION

Carbon nanotubes (CNTs) have been amongst the most-studied nanomaterials,[1] with recent applications in nanoelectromechanical systems (NEMS).[2,3] Due to their combination of high stiffness and low weight, CNTs have been investigated for NEMS-based sensing applications, with a particular interest in ultrasensitive mass sensing[4,5] and force sensing.[6,7]

For enhanced sensitivity to environmental (i.e., forces and masses) changes, the quality (Q)-factors of NEMS are of particular interest. In particular, high Q-factors are desired for NEMS applications as this indicates smaller energy dissipation per vibrational cycle, or equivalently smaller linewidths during the resonance of the NEMS. Regardless of the physical interpretation, higher Q-factors lead to greater sensitivity and resolution of adsorbed masses or surrounding forces, and thus are highly desired.

The resonance, and Q-factors of both fixed/free,[4,8] and fixed/fixed[3,9–12] CNT oscillators have been studied experimentally by various researchers. Q-factors ranging from 15[9] to 1000[4] were found. Particularly relevant to the present work is the study of Purcell et al.,[11] who applied tension to the CNTs using an electric field, thereby tuning the resonant frequency of the CNT; they reported Q-factors as high as 2500, though the dependence of Q with tensile strain was not discussed. More recently, Q-factors as high as 10^5 were found by Huttel et al.[12] in fixed/fixed carbon nanotubes.

The nature of the boundary conditions that are used to fix or clamp the ends of the CNTs during resonance are of interest for various reasons, though a comprehensive experimental study delineating the effects of boundary condition, i.e., fixed/free versus fixed/fixed ends on the Q-factors of the CNTs has not been performed. The boundary condition is important for the following reasons. First, fixed/free nanotubes will have a higher dynamic range,[4] which means that they can undergo larger deformations before nonlinear effects are excited. Furthermore, extrinsic clamping losses[13] through interaction with the fixed substrate will be minimized for fixed/free boundary conditions, due to being clamped at only one end.

In contrast, while fixed/fixed nanotubes may suffer enhanced extrinsic clamping losses, evidence exists that, because mechanical strain can more easily be applied experimentally in the fixed/fixed configuration, that the Q-factors of various nanostructures, including metal nanowires,[14] graphene monolayers,[15] silicon and silicon nitride nanowires,[16,17] MEMS heterostructures[18] and carbon nanotubes[19] can be tuned and, more importantly, enhanced through the application of tensile mechanical strain.

Energy dissipation in oscillating CNTs has been studied using classical molecular dynamics (MD) for both single

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1546-1955/2011/8/814/006 doi:10.1166/jctn.2011.1758

walled (SW) CNTs,[20] and multi walled (MW) CNTs,[20-22] and more recently for graphene mono and multilayers.[15,23] Of these, Jiang et al.[20] studied the temperature dependence of Q-factor degradation in both fixed/free SWCNTs and MWCNTs, while other works[21,22] focused on frictional effects on energy dissipation in MWCNTs.

Therefore, the purpose of the present work is to utilize classical MD to study the following. First, we will determine the effects of boundary condition on the intrinsic Q-factors of single-walled CNTs. Second, we will determine the utility of mechanical strain in enhancing the intrinsic Q-factors of fixed/fixed CNTs, where by focusing on intrinsic loss mechanisms, i.e., due to thermoelastic dissipation,[24] we neglect extrinsic energy loss mechanisms such as gas damping effects and clamping losses on the CNT Q-factors.

2. SIMULATION DETAILS

Classical MD simulations were performed on (5,5) fixed/fixed single-walled CNTs, where both ends of the CNT were fixed. The (5,5) fixed/fixed CNT had 240 carbon atoms and a length of 28.37 Å, which is identical to the single-walled CNT considered by Jiang et al.[20]

We utilized the second generation Brenner potential (REBO-II)[25] for the carbon–carbon interactions; this potential has been shown to accurately reproduce binding energies, force constants and elastic properties of graphene. For all simulations, the CNT was first equilibrated at a specified temperature using a Nose-Hoover thermostat[26] for 100000 steps with a 1 femtosecond (fs) time step within an NVT ensemble. After the initial thermal equilibration, a sinusoidal velocity was applied to the CNT which caused the CNT to oscillate; the oscillation was performed within an energy-conserving NVE ensemble. The velocity profile was zero at the fixed ends of the CNT, and sinusoidally increased to a maximum at the center of the CNT, which caused the magnitude of oscillation of the center of the CNT to be about 0.70 Å, which is about 2.47% of the length of the CNT. We emphasize that the energy of the CNT increased only 1.16 eV (compared to an original energy of 1695 eV) due to the imposed sinusoidal velocity profile, or less than 0.1% of the total energy of the CNT, such that nonlinear vibrational effects would not be spuriously introduced in the simulations.

We performed simulations only on fixed/fixed CNTs in the present work, as results for the Q-factors of fixed/free CNTs were obtained in a 2004 paper by Jiang et al.[20] A direct comparison between the fixed/fixed geometries in the present work to the fixed/free results of Jiang et al. is feasible as Jiang et al. used not only the same potential (REBO-II), but also the same geometry, i.e., (5,5) CNTs with 240 atoms. Therefore, we are able to isolate boundary condition effects as the cause of any differences between the Q-factors reported here for fixed/fixed (5,5) CNTs and the fixed/free (5,5) CNTs reported by Jiang et al.[20]

3. RESULTS

3.1. Boundary Condition Effects on Q

We first discuss the effect of boundary condition on the Q-factors of the CNTs. Again, we have calculated only the fixed/fixed (5,5) single-walled CNTs; the data for comparison was taken from the identical (5,5) fixed/free CNTs of Jiang et al.[20]

Similar to Jiang et al.,[20] we show in Figure 1 the external energy (EE) time history for the fixed/fixed (5,5) CNT at different temperatures, ranging from 0.05 K to

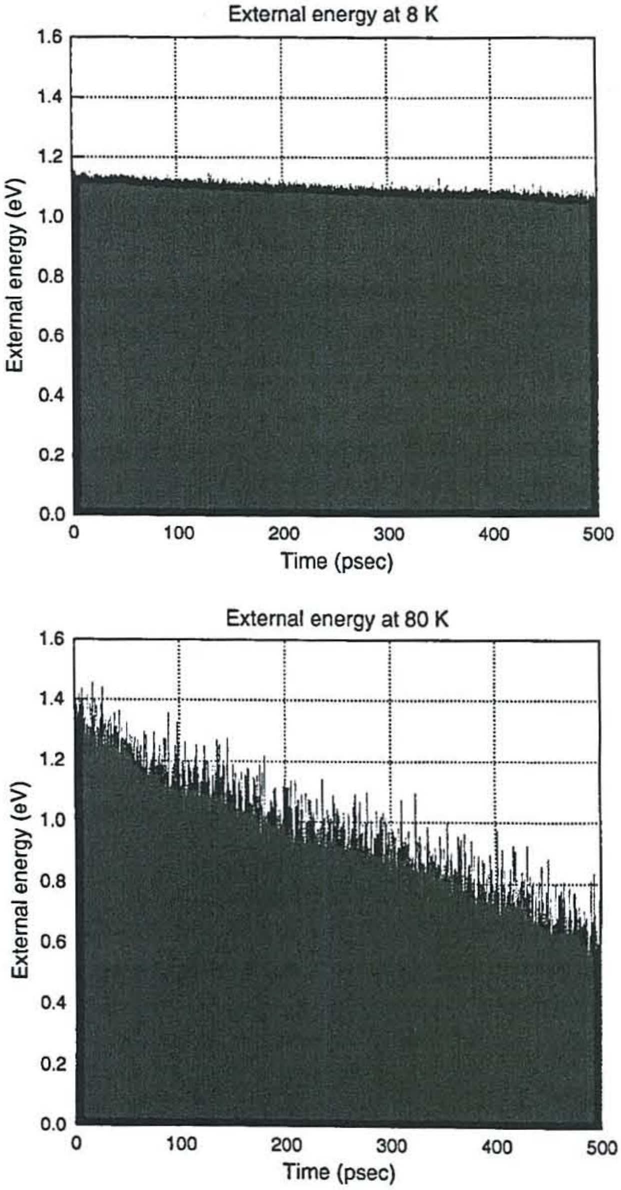

Fig. 1. Intrinsic energy dissipation for fixed/fixed CNT at different temperature, no applied strain.

293 K. We note that the EE is defined as the difference of the potential energy (PE) before and after the sinusoidal velocity profile, which causes the subsequent oscillation of the CNT, is applied.

As can be seen in Figure 1, the energy dissipation clearly increases with an increase in temperature, which demonstrates the thermoelastic dissipation that is characteristic in oscillating structures. We further quantify the nature of the temperature-dependent energy dissipation by plotting in Figure 2 the Q-factor versus temperature for both fixed/fixed and fixed/free (5,5) CNTs.

The first trend we note is that, particularly at low temperatures, the Q-factors of fixed/fixed CNTs are significantly higher than those of fixed/free CNTs; for example, at 1 K, the Q-factors of fixed/fixed CNTs are about 360,000, while the Q-factors of fixed/free CNTs are about 13,000, for an increase in Q of nearly a factor of 30 simply by changing the boundary condition.

Despite the significant increase in Q-factor at low temperatures, Figure 2 demonstrates that, as temperature increases, the Q-factors of fixed/fixed CNTs degrade more quickly than do the Q-factors of fixed/free CNTs. Thus, at 293 K, the Q-factor of the fixed/fixed CNT has reduced to 2200, while the Q-factors of the fixed/free CNT reduce to about 1500. The reason for this is due to their different exponent which relates the Q-factor and temperature. For example, Jiang et al.[20] determined that $Q \approx 1/T^{0.36}$ for fixed/free CNTs. In the present work, we determine for fixed/fixed CNTs that the relationship between Q-factor and temperature is $Q \approx 1/T^{0.91}$.

The exponent relating Q-factor and temperature is different between fixed/fixed and fixed/free boundary conditions for one key reason. Before discussing this, we note that the exponent of 0.91 for the fixed/fixed CNTs is essentially the same as the thermoelastic damping exponent of 1.0 that is expected for bulk materials.[27] The exponent of 0.36 for the fixed/free CNTs obtained by Jiang et al.[20] reflects the fact that fixed/free CNTs have one unrestrained end where the carbon atoms at the unfixed end have dangling bonds; these dangling bonds induce a surface effect which causes the thermoelastic damping exponent to deviate sharply from the bulk value. In contrast, all undercoordinated atoms at the ends of the CNT are fixed in the fixed/fixed CNTs; because of this, all surface effects have been removed, which causes the thermoelastic damping exponent to essentially mimic that of a bulk material.

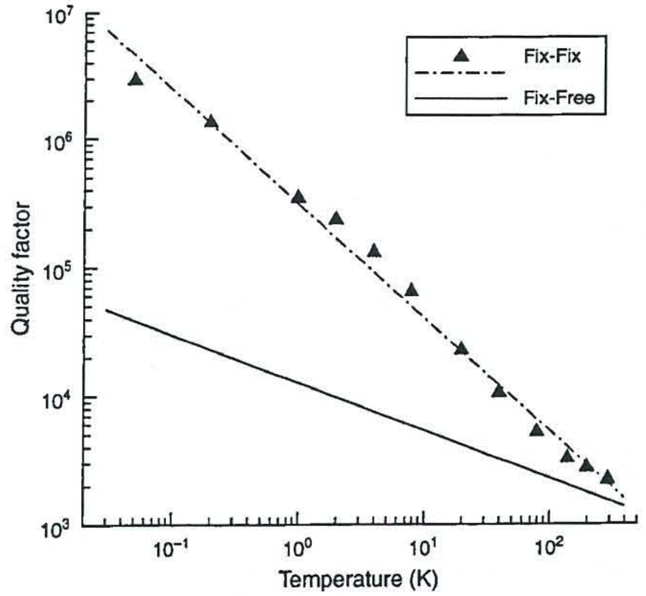

Fig. 2. Q-factor as a function of temperature and boundary condition for CNTs; fixed-free data taken from Jiang et al. Reprinted with permission from [20], H. Jiang et al., *Phys. Rev. Lett.* 93, 185501 (2004). © 2004, American Physical Society.

3.2. Strain Effects on Q-Factors of Fixed/Fixed CNTs

The results of the previous section suggest that there may be advantages to using fixed/fixed CNTs for low-temperature NEMS applications, while the situation is less clear at realistic operating temperatures like room temperature, both due to the similarity in Q-factor, and also due to the fact that extrinsic damping losses, like gas damping, have not been considered.

However, as discussed in the introduction, one advantage of the fixed/fixed configuration is that it is possible experimentally to impose strain, both tensile and compressive, on the CNT or other nanostructures, as has been demonstrated by various researchers.[11, 17, 18, 28] Furthermore, because mechanical strain, and in particular tensile mechanical strain has been successfully utilized in the past to enhance the Q-factors of various nanostructures,[14, 15, 17, 18] including carbon-based nanostructures such as graphene,[15] we now investigate the effect of strain on the Q-factors of fixed/fixed CNTs.

To study the Q-factors of fixed/fixed CNTs under strain, we follow a similar procedure as described previously, except that first, the CNT is stretched uniaxially under either tension or compression with strain increments of 1% to the desired tensile or compressive strain state at 0 K following an energy minimization algorithm. At that point, the CNT is equilibrated at the desired temperature, and then the sinusoidal velocity field is applied in order to cause the CNT to oscillate.

Figure 3 illustrates the effect of applied tensile and compressive strain on the Q-factors of fixed/fixed CNTs at the same temperature. In particular, it demonstrates the significantly different response in energy dissipation at 20 K at different levels of strain. It is clearly observed that there is significantly less energy dissipation at 5% tensile strain than at 3% compressive strain. This result is consistent with previous studies on metal nanowires[14] and graphene monolayers[15] where tensile strain was also found to mitigate intrinsic energy dissipation.

To quantify the effects of tensile and compressive strain on the Q-factors of fixed/fixed CNTs as a function of

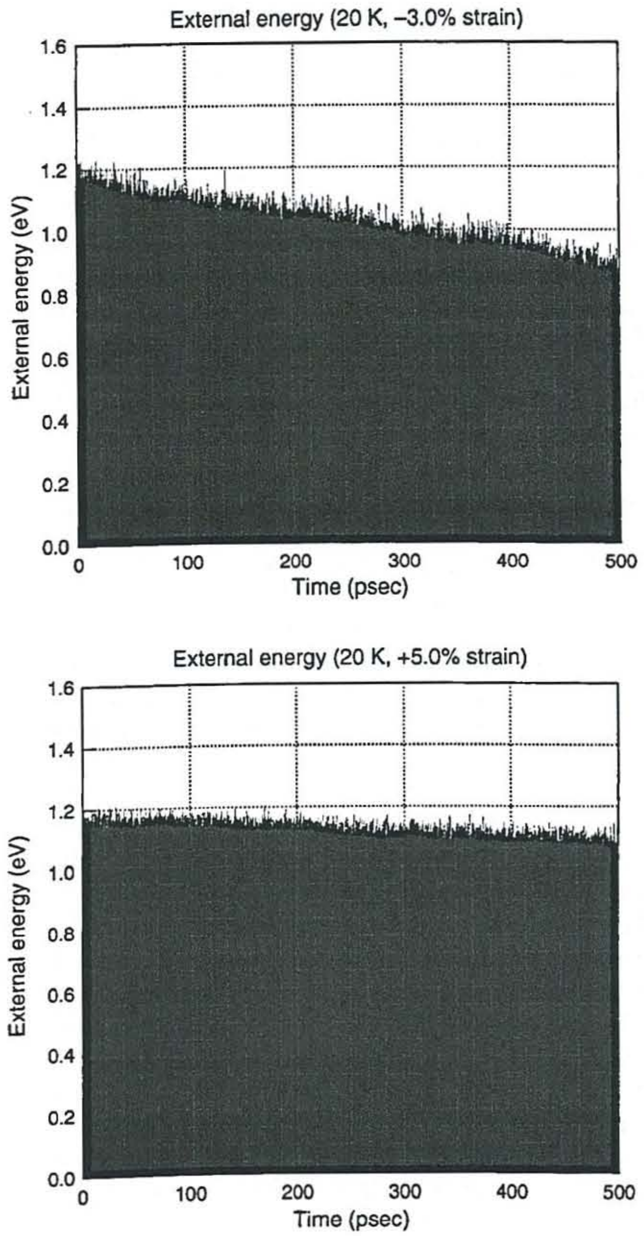

Fig. 3. Intrinsic energy dissipation for fixed/fixed CNT at same temperature, different amounts of applied tensile or compressive strain.

temperature, we plot in Figure 4 the Q-factors as a function of strains ranging from 4% compressive to 6% tensile for temperatures ranging from 1 K to 140 K. It can be observed that for all temperatures, there is a nearly linear increase in Q-factor with applied tensile strain; however, further inspection of Figure 4 also indicates that, with increasing temperature, the linear constant of Q enhancement also decreases.

To quantify this further, we assume a linear relationship between Q-factor and strain for a given temperature as

$$Q = A\epsilon Q_0 \tag{1}$$

where ϵ is the imposed strain, Q_0 is the Q-factor for a given temperature at 0% applied strain, and A is an

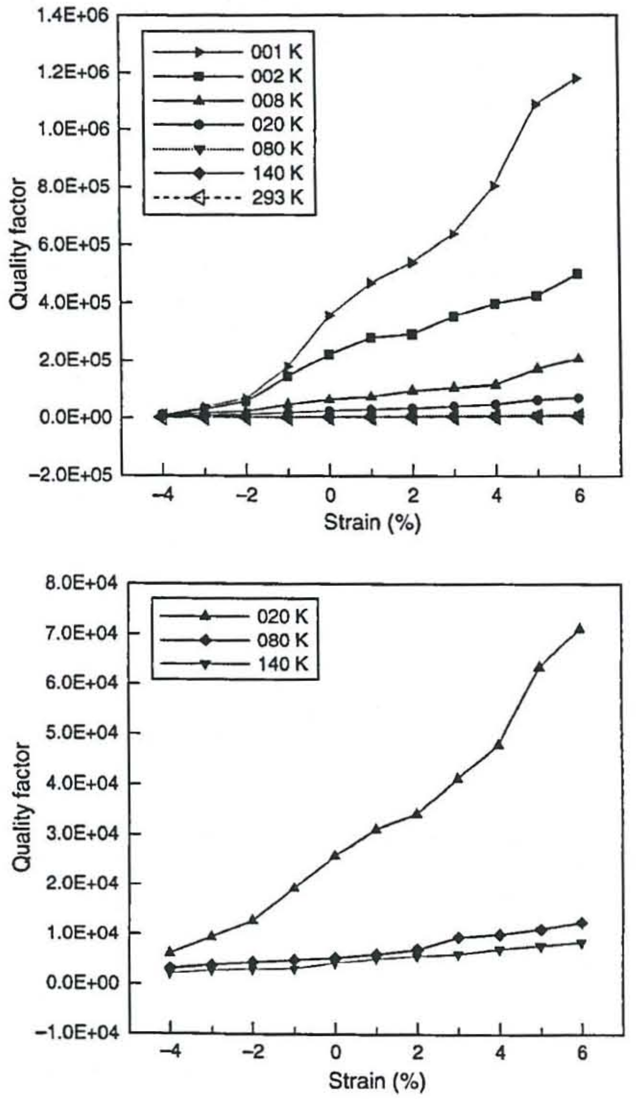

Fig. 4. (Top) Q-factor as a function of temperature and strain for fixed/fixed CNT. (Bottom) Extended view to delineate the Q-factor variation with temperature and strain.

unknown constant that depends upon the temperature. In Table I, we list the Q-factors for various temperatures as a function of strain, and also give the constant A.

As can be seen, while the approximately linear relationship holds across the range of temperatures between Q-factor and tensile strain, the constant A decreases significantly with an increase in temperature from $A = 0.55$ at

Table I. Q-factors as a function of strain and temperature for fixed/fixed (5,5) single-walled CNT. Also gives the constant A in the equation $Q = A\epsilon Q_0$.

T (°K)	Q_0 (0% Strain)	Q (3% Strain)	Q (6% Strain)	A
1	360,000	640,000	1,200,000	0.55
8	66,000	110,000	210,000	0.53
20	24,000	41,000	71,000	0.49
140	3,400	6,100	8,400	0.41
293	2,200	2,600	3,200	0.24

1 K to $A = 0.24$ at 293 K. This indicates that while tensile strain does increase the Q-factors of fixed/fixed CNTs at elevated temperatures, its effectiveness diminishes with an increase in temperature.

It is also relevant to discuss the amount of tensile strains we have considered in the present work. The maximum tensile strain we applied was 6%; for comparison, previous MD simulations by Belytschko et al.[29] of the tensile loading of single walled carbon nanotube found failure strains ranging from 10–15%. Overall, these results indicate that the amount of tensile strain (0–6%) we have utilized in the present work should not lead to any instabilities or defects in the fixed/fixed CNT.

We close by discussing two items. First, we discuss Figure 5, where we plot the dependence of the Q-factor on temperature and both tensile and compressive strain. What is most interesting about Figure 5 is that regardless of the amount of tensile strain that is applied to the fixed/fixed CNT, the thermoelastic damping exponent remains constant at 0.91, i.e., $Q \approx 1/T^{0.91}$. Finally, we note that when compressive strain is applied, the thermoelastic damping exponent decreases dramatically, with a decrease in exponent with an increase in strain.

Second, an interesting future research path concerns the application of tensile strain, and the effects on the Q-factors of MWCNTs. As shown by Jiang et al.[20] for MWCNTs, and by Kim and Park for multilayer graphene,[23] frictional interactions between the carbon layers cause a significant decrease in the Q-factors of these multi-walled or multilayer structures. It seems likely that tensile strain will improve the Q-factor degradation due to these interlayer frictional effects, though the nature of the effect and the factors controlling it has not been quantified to-date.

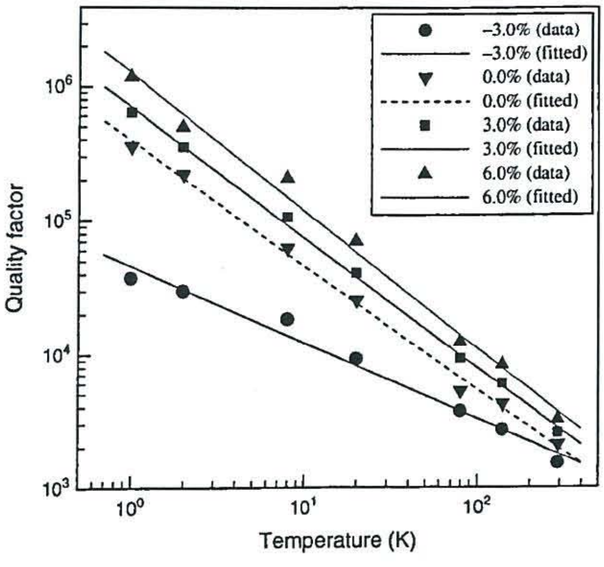

Fig. 5. Q-factor as a function of temperature and strain for fixed/fixed CNT.

4. CONCLUSIONS

In conclusion, we have utilized classical MD to study boundary condition and strain effects on the Q-factors of single-walled CNTs. We have found that, excluding extrinsic damping effects, fixed/fixed CNTs generally have higher Q-factors than do fixed/free CNTs, though the difference in Q-factor due to boundary condition decreases with increasing temperature. We further demonstrated that the Q-factors of fixed/fixed CNTs can be enhanced by factors of 2–4 through the application of tensile mechanical strain, though again, the effectiveness of the Q-factor enhancement decreases with increasing temperature. The results collectively indicate that fixed/fixed CNTs should be preferable for NEMS applications at lower temperatures due to a combination of their inherently higher Q-factors, and the fact that the Q-factors can be further improved through application of tensile strain. However, near room temperature, with mechanical strain, the intrinsic Q-factors of fixed/fixed CNTs are about double those of fixed/free CNTs, which may or may not be sufficient to overcome the loss in Q-factors that result due to the increase in extrinsic damping for fixed/fixed nanostructures.

Acknowledgments: Sung Youb Kim and Harold S. Park both gratefully acknowledge the support of DARPA through grant HR0011-08-1-0047. The authors note that the content of this article does not necessarily reflect the position or the policy of the government, and that no official government endorsement of the results should be inferred. HSP also acknowledges support from NSF grant CMMI-0750395.

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Received: 13 September 2009. Accepted: 10 January 2010.