Modeling and Simulation on Crossroad-Type Graphene-Resonator Accelerometer

Oh Kuen Kwon[*] and Jeong Won Kang[**]

[*]Department of Electronic Engineering, Semyung University, Jecheon 12136, Republic of Korea, kok1027@semyung.ac.kr
[**]Graduate School of Transportation, Korea National University of Transportation, Uiwang-si 16106, Republic of Korea, jwkang@ut.ac.kr

ABSTRACT

Highly sensitive accelerometers have multiple applications in industry and science, and can be used as sensors in a wide variety of devices. Here, we investigate the application of crossroad-type graphene resonators as ultrahigh sensitivity accelerometers by performing classical molecular dynamics simulations. The relationships between the resonance frequencies and acceleration could be divided by two regions. The simulation data showed that when the accelerations were higher than 0.1 nm/ps^2, the resonance frequency increased with increase of the acceleration. In particular, acceleration, as a function of frequency, was regressed by a power function and shown to have a linear relationship on a log-log scale. Crossroad-type graphene resonators have multiple applications to nanoscale sensors, filters, switching devices, and quantum computing, as well as ultra-fast response resonators.

Keywords: graphene resonator, acelerometer, crossroad-type graphene, molecular dynamics

1 INTRODUCTION

Since its discovery, graphene,[1-4] pure carbon in the form of a very thin, nearly transparent sheet of one atom in thickness, has attracted a great deal of attention due to its extraordinary electronic and mechanical properties.[5-10] Recent research has led to the development of high-frequency top-down fabricated mechanical resonators based on graphene.[5-7] Nanoelectromechanical system (NEMS) resonators, which provide high frequency resolution and long energy storage time, play an important role in many fields of science and engineering.[11] Thus, graphene has recently come to be regarded as the basic element of NEMS devices, due to its unique mechanical properties.[5-7]

Accelerometers have multiple applications in industry and science, and can be used as sensors in a wide variety of devices. Highly sensitive accelerometers are components of inertial navigation systems for both aircraft and missiles, as these predominantly require guidance, navigation, and control applications. Accelerometers can be used to detect and monitor vibration in rotating machinery, tablet computers and digital cameras, allowing images on the screens to always be displayed upright, as well as in drones for flight stabilization. New technologies have resulted in the continuous advancement of inertial measurement systems.[12,13] Efforts in recent years have been directed towards the realization of increasingly smaller rotation-rate sensors with lower power requirements, capable of achieving performance commensurate with the requirements for non-GPS navigation of small platforms.[14] In particular, graphene based accelerometers have great advantages in terms of providing a large sensing range, reproducibility of performance without hysteresis, and stability in mechanical operation.[15] This has caused intense investigation into resonators based on graphene nanoribbon.[5-10]

In our previous work,[16] crossroad-type graphene-based resonators were addressed. We presented simple fabrication schematics for a crossroad-type graphene resonator and analyzed its dynamic features via classical molecular dynamics (MD) simulations. The metal was deposited on insulator film and then a hole was formed through selective etching processes after masking. The graphene was then transferred onto the bottom plate. Suspended graphene sheets were fabricated with a peeling process similar to that reported previously.[5] In our schematics, the graphene sheet could be mechanically exfoliated over a predefined hole etched into a SiO_2 surface.[5] A cross-type mask pattern is then formed on the graphene through the process of fine lithography.

In the present work, we consider a crossroad-type graphene resonator as an accelerometer, and investigate its dynamic properties via classical MD simulations. The relationships between the resonance frequencies and acceleration could be divided by two regions. Data from the MD simulations showed that for accelerations higher than 0.1 nm/ps^2, the resonance frequency increased with the increase in acceleration. In particular, acceleration, as a function of frequency, was regressed by a power function and shown to have a linear relationship on a log-log scale.

2 SIMULATION METHODS

The simulation structure for the crossroad-type graphene resonator, which was composed of 1120 atoms, is presented in Figure 1. The lengths of the zigzag and armchair directions were 11.8 nm and 12.0 nm, respectively. Atoms on the four edges were fixed during the MD simulations. The MD simulations for the crossroad-type graphene resonator were performed under applied driving force (F_A), which was equally distributed over the resonator, and then the resonator was actuated. Variations of the center deflections and the resonance frequencies for the driving forces were observed as acceleration occurred. The MD simulations were performed with different driving forces, ranging from 0.01792 to 17.92 nN.

To investigate the dynamics of the crossroad-type graphene resonator, the MD simulations were performed using the MD methods from previous studies.[15,16] The in-house MD code used the velocity Verlet algorithm and neighbor lists for improvement of the computing performance. The MD time step (Δt) was 5×10^{-1} or 5×10^{-4} ps. The temperatures in all MD simulations were set to 1 K, and the total MD times were 1 ns. To describe the carbon-carbon interactions in the crossroad-type graphene resonator, the Tersoff–Brenner potential function was employed,[17-19] which has been widely applied in carbon systems.

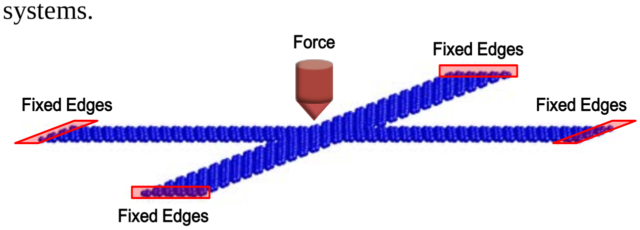
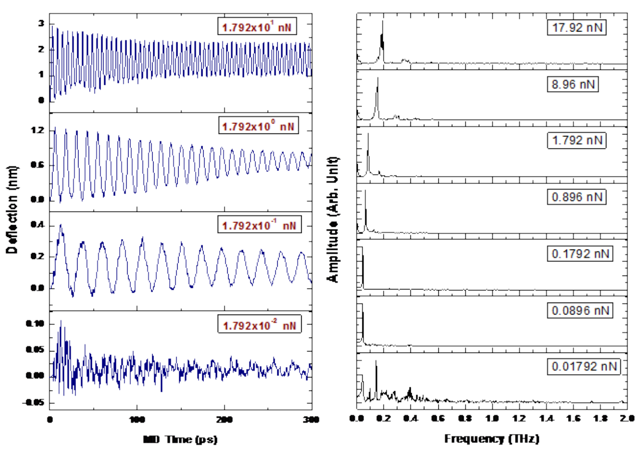


Figure 1. Simulation structure of the crossroad-type graphene resonator.



(a) (b)

Figure 2. (a) Variation in center deflection as a function of the MD time. (b) Normalized amplitude spectra as a function of the frequency for different applied forces.

3 RESULTS AND DISCUSSION

Figure 2(a) shows the center deflection variations as a function of the MD time for F_A = 0.01792, 0.1792, 1.1792, and 17.92 nN. Since the driving force was abruptly applied to the crossroad-type graphene resonator in the beginning, the deflections were high during the early stage. However, as the MD time increased, the deflections were gradually dampened by dissipating kinetic energy, and stabilization occurred. The plots clearly showed the vibrating crossroad-type graphene resonator under externally applied forces.

Using the data from Figure 2(a), the spectra for different applied forces can be obtained from the fast Fourier transformation (FFT) calculations, as displayed in Figure 2(b), which demonstrate the normalized amplitude spectra as a function of the frequency for different applied forces. Some trends of the resonance frequencies against the applied forces could be found. Figure 3 shows the resonance frequencies as a function of the deflection. In this plot, three cases of deflections were considered, including the mean deflections obtained by the FFT calculations, the centers of the deflections obtained from the MD simulations, and the maximum deflections obtained from the MD simulations. Except for very small deflections, the resonance frequencies increased almost linearly with increase of the deflections. Practically, since the maximum displacements of the crossroad-type graphene resonators are very difficult to detect in actual systems, the mean deflections as a time-dependent average value, which can be obtained from real-time sensing data, will provide important information to sense the deflections of the resonators.

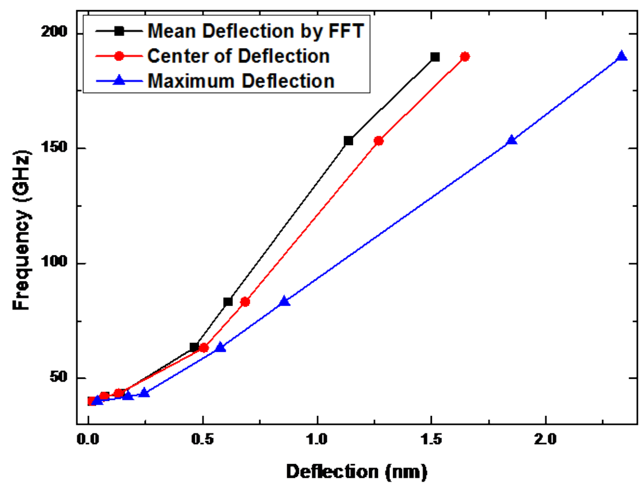
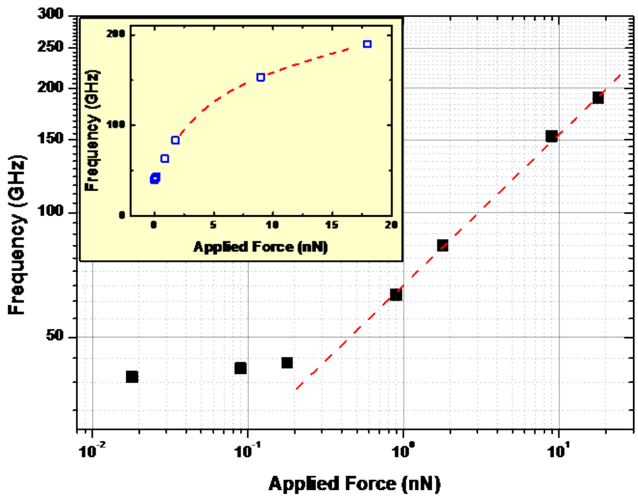


Figure 3. Resonance frequencies as a function of the deflection.

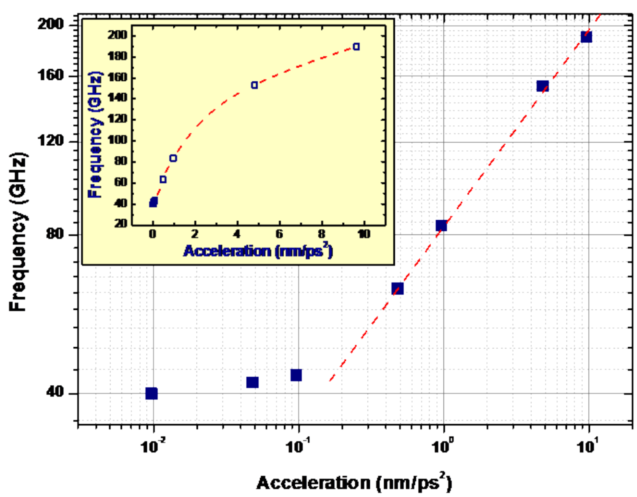
The resonance frequencies (f) as a function of the applied force (nN) and the acceleration (nm/ps^2) in *log-log* scale are shown in Figures 4(a) and 4(b). These plots show two regions in the relationship between resonance frequencies and acceleration. When the applied forces were higher than 0.2 nN, the resonance frequency increased with increase of the externally applied force; then, log(f) ~ log(F_A). In this work, when the accelerations were higher than 0.1 nm/ps^2, the resonance frequency increased with increase in the acceleration. The acceleration-frequency relationship was very clear on the *log-log* scale. Such a result is quite similar to the results obtained for GNR-resonators when used as mass sensors.[20]

The non-linearity of the GNR-resonators increases with increasing initial strain as well as increasing applied force.[20]

Typically, GNR-resonators undergo non-linear operation in the presence of large strain.[21-23] Such non-linear mechanical properties of the GNRs were in good agreement with the previous work by Georgantzinon *et al.*[22,23] The MD simulations performed by Bu *et al.*[21] also showed that GNRs behave non-linear elastically under tensile loads. Such non-linearity of the GNR-resonator under large externally applied accelerations is very important to understanding its operating dynamics and the changes of sensitivity and sensing range.



(a)



(b)

Figure 5. Resonance frequencies as a function of (a) the applied force (nN) and (b) the acceleration (nm/ps^2) in a log-log scale.

The simulation results obtained herein presented the dynamic features of the crossroad-type graphene resonators applicable to ultrahigh sensitive accelerometers by sensing the frequency shift. In this work, all MD simulations were performed at extremely low temperature, so the dynamics features of the accelerometer were only examined in ideal situations. However, the results obtained herein are meaningful in terms of providing information on the operation of accelerometers even when thermal effects are also considered, for example, by noting the fact that the quality factors of the GNR-resonators were greatly decreased by increasing temperature.[6] In practice, temperature fluctuation influences the vibrational behavior of graphene resonators. Hüttel et al.[24] showed that the operating temperature affected the non-linearity and quality factor of CNT-resonators. The response of CNT-resonators changed from non-linear to linear when the operating temperature was increased, and the temperature increase also resulted in a decrease in the quality-factor as a power law.[24] Chen et al.[6] investigated GNR-resonators with a high quality factor of ~1×10^4, and found the quality factor to increase with decreasing temperature.[24] The sensing range, sensitivity and reliability are very closely related to the dimensions of the graphene-nanoribbon-resonator and environmental effects.

The present work demonstrated that a graphene resonator with crossroad-type structure demonstrates great potential for application in the detection of acceleration. Especially, crossroad-type graphene has both types of edges such as zigzag and armchair, and since the electrical properties of the zigzag direction are hardly different from those of the armchair direction, the electromechanical couplings for both directions can be detected at the same time. This property can allow the crossroad-type graphene resonator to sense quantum phenomena. The high frequency NEMS resonator can offer not only the potential for extreme mass and force sensitivity, but also a unique way to directly observe the imprint of quantum phenomena, including investigation of the uncertainty principle limits on position detection.[25] Therefore, the polarization of the crossroad-type graphene resonator can also provide a graphene-nanoribbon-based quantum-computer for quantum-mechanical coupling, as well as mass detectors, accelerometers or alarms.

Finally, it should be noted that the mechanical quality factor also plays a very important role in determining the sensitivity of NEMS devices. However, this is not discussed in the present work. The entire study was based on the temperature of 1 K for all MD simulations, which is extremely low and highly unrealistic. Therefore, further work should include MD simulations carried out at a range of temperatures substantially higher than 1 K in order to take into account thermal dissipation, as experiments are most likely to be conducted at temperatures much larger than 1 K. One can expect that the quality factor will be greatly decreased by increasing temperature, as found in studies regarding the cantilevered CNT beam oscillator by Jiang *et al.*[26] and on graphene resonators by Chen *et al.*[6] It is clear that the frequency range and sensing ability of the crossroad-type graphene resonators are dependent on structural parameters and experimental setup. Therefore, such issues need to be addressed in further works by considering several situations, as well as the mechanical and thermal properties of graphene in detail. Moreover, further works should include quantum mechanics to reveal

TechConnect Briefs 2017, TechConnect.org, ISBN 978-0-9988782-1-8

the electronic properties of unusual carbon nanostructures,[27-29] electron transport properties,[30-32] and the influences of electric and magnetic fields,[33-35] as well as the structural and mechanical properties.[36]

4 CONCLUDING REMARKS

We presented application of the suspended crossroad-type graphene resonator as an accelerometer, for which the dynamic properties were investigated via classical MD simulations. The deflective motions of the crossroad-type graphene resonator under driving forces were very similar to those of the graphene-nanoribbon resonator. Our simulations data showed that the relationships between the resonance frequencies and the acceleration could be divided by two regions. For accelerations greater than 0.1 nm/ps^2, the resonance frequency increased with increasing acceleration. In particular, the acceleration-frequency relationship was very clear on the log-log scale. The crossroad-type graphene resonators have multiple applications to nanoscale sensors, filters, switching devices, and quantum computing, as well as ultra-fast response resonators.

ACKNOWLEDGMENTS: This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future planning (2015R1A1A1A05027643), and the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (2014H1C1A1066414).

REFERENCES

[1] H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).
[2] K. Geim Science 324, 1530 (2009).
[3] Y. Zhang, Y.-W. Tan, H. L. Stormer, P. Kim, Nature 438, 201 (2005).
[4] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, A. A. Firsov, Nature 438, 197 (2005).
[5] J. S. Bunch, A. M. van der Zande, S. S. Verbridge, I. W. Frank, D. M. Tanenbaum, J. M. Parpia, H. G. Craighead, P. L. McEuen, Science 315, 490 (2007).
[6] Chen, S. Rosenblatt, K. I. Bolotin, W. Kalb, P. Kim, I. Kymissis, H. L. Stormer, T. F. Heinz, J. Hone, Nat. Nanotechnol. 4, 861 (2009).
[7] Garcia-Sanchez, A. M. van der Zande, A. San Paulo, B. Lassagne, P. L. McEuen, A. Bachtold, Nano Lett. 8, 1399 (2008).
[8] Lee, X. Wei, J. W. Kysar, J. Hone, Science 321, 385 (2008).
[9] Gomez-Navarro, M. Burghard, K. Kern, Nano Lett. 8, 2045 (2008).
[10] J. Atalaya, A. Isacsson, J. M. Kinaret, Nano Lett. 8, 4196 (2008).
[11] R. Poncharal, Z.L. Wang, D. Ugarte, W.A. de Heer, Science 283, 1513 (1999).
[12] R. Ragan, IEEE Trans. Aerosp. Electron. Syst. 20, 414 (**1984**).
[13] R. Dixon and J. Bouchaud, WTC-Wicht Technologie Consulting: Think Small 1, 1 (**2006**).
[14] T. Clark and C. Nguyen, CINT-Database of Government Nanotechnology Programs. Program ID 04-00946 and Solicitation Number BAA05-02 (**2004**).
[15] J. W. Kang, J. H. Lee, H. J. Hwang, K.-S. Kim, Phys. Lett. A 376, 3248 (2012).
[16] O. K. Kwon, H. J. Hwang, and J. W. Kang, Comput. Mater. Sci. 82, 280 (2014).
[17] J. Tersoff, Phys. Rev. B 38, 9902 (1988).
[18] J. Tersoff, Phys. Rev. B 39, 5566 (1989).
[19] D.W. Brenner, Phys. Rev. B 42, 9458 (1990).
[20] K.-R. Byun, K.-S. Kim, H. J. Hwang, and J. W. Kang, J. Comput. Theor. Nanosci. 10, 1886 (2013).
[21] H. Bu, Y. Chen, M. Zou, H. Yi, K. Bi, Z. Ni, Phys. Lett A 373, 3359 (2009).
[22] S. K. Georgantzinos, G. I. Giannopoulos, D. E. Katsareas, P. A. Kakavas, N. K. Anifantis, Computat. Mater. Sci. 50, 2057 (2011).
[23] S. K. Georgantzinos, D. E. Katsareas, N. K. Anifantis, Physica E 43, 1833 (2011).
[24] A. K. Hüttel, G. A. Steele, B. Witkamp, M. Poot, L. P. Kouwenhoven, and H. S. J. van der Zant, Nano Lett. 9, 2547 (2009).
[25] K. C. Schwab, M. L. Roukes, Physics Today 58, 36 (2005).
[26] H. Jiang, M.-F. Yu, B. Liou, Y. Huang, Phys. Rev. Lett. 93, 185501 (2004).
[27] P. K. Bose, N. Paitya, S. Bhattacharya, D. De, S. Saha, K. M. Chatterjee, S. Pahari, and K. P. Ghatak, Quantum Matter 1, 89 (2012).
[28] B. Tüzün and C. Erkoç, Quantum Matter 1, 136 (2012).
[29] T. Ono, Y. Fujimoto, and S. Tsukamoto, Quantum Matter 1, 4 (2012).
[30] M. Narayanan and A. J. Peter, Quantum Matter 1, 53 (2012).
[31] N. Paitya, S. Bhattacharya, and K. P. Ghatak, Quantum Matter 1, 63 (2012).
[32] A. Khrennikov, Rev. Theor. Sci. 1, 34 (2013).
[33] A. Herman, Rev. Theor. Sci. 1, 3 (2013).
[34] E. L. Pankratov and E. A. Bulaeva, Rev. Theor. Sci. 1, 58 (2013).
[35] Q. Zhao, Rev. Theor. Sci. 1, 83 (2013).
[36] J. W. Kang and K. W. Lee, Nanosci. Nanotechnol. 14, 9158 (2014).