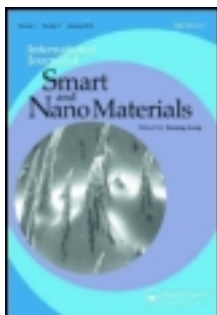


This article was downloaded by: [George Washington University], [Xianqiao Wang]  
On: 06 December 2011, At: 07:48  
Publisher: Taylor & Francis  
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered  
office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



## International Journal of Smart and Nano Materials

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/tsnm20>

### Simulation of collisions between buckyballs and graphene sheets

Zhen Zhang<sup>a</sup>, Xianqiao Wang<sup>a</sup> & Jiaoyan Li<sup>a</sup>

<sup>a</sup> Department of Mechanical and Aerospace Engineering, The George Washington University, Washington, DC, 20052, USA

Available online: 06 Dec 2011

To cite this article: Zhen Zhang, Xianqiao Wang & Jiaoyan Li (2011): Simulation of collisions between buckyballs and graphene sheets, International Journal of Smart and Nano Materials, DOI:10.1080/19475411.2011.637993

To link to this article: <http://dx.doi.org/10.1080/19475411.2011.637993>



PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.tandfonline.com/page/terms-and-conditions>

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

## Simulation of collisions between buckyballs and graphene sheets

Zhen Zhang, Xianqiao Wang\* and Jiaoyan Li

Department of Mechanical and Aerospace Engineering, The George Washington University,  
Washington, DC 20052, USA

(Received 2 August 2011; revised version received 2 November 2011)

The phenomena of buckyball–graphene collisions were investigated by classical molecular dynamics (MD) simulation using the empirical Tersoff potential. Three cases were investigated: collisions between a buckyball and a single-layer graphene; collisions between a nano-onion (a double-layer concentric spherical nanostructure: a  $C_{60}$  in a  $C_{320}$ ) and a single-layer graphene; collisions between a nano-onion and a double-layer graphene. The impact velocity of the buckyball or nano-onion ranged from 4.37 km/s to 15.31 km/s. Simulation results for the buckyball–graphene collisions show that the buckyball bounces back when the impact velocity is less than 8.75 km/s, sticks to the graphene when the impact velocity is between 8.75 km/s and 12.03 km/s, and breaks when the impact velocity is greater than 12.03 km/s. Similar phenomena are observed for the other two cases. A single buckyball can never go through a single-layer graphene intact; however, the inner structure ( $C_{60}$ ) of a nano-onion can penetrate through a single-layer graphene without any damage. The energy evolution during the whole simulation process was also studied.

**Keywords:** graphene; buckyball; nano-onion; collisions; Tersoff potential

### 1. Introduction

Graphene, a two-dimensional material system and the building block of fullerenes, carbon nanotubes, and graphite, is not only the thinnest material in the universe, but also the strongest material ever tested [1,2]. Its extraordinary peculiarities in mechanical, electronic, thermal, and optical aspects [1,3–9] drive to the use of graphene for many applications, especially for nanoelectromechanical systems (NEMS) [10], base materials for electronic circuitry [11], and biodevices [12]. Recently, researchers have found that  $C_{60}$  buckyballs can be used to make graphene quantum dots that are geometrically well defined [13]. However, there are relatively few works that have been performed on the modeling of mechanical characteristics of graphene, especially on the behavior of the graphene sheets under collisions with other molecules. The damage of graphene and its resistance under high-energy collisions is an important consideration in some potential applications, like offensive and defensive weapons (spear-shield) in future warfare.

Surface interactions of buckyballs with different kinds of materials, such as silicon, diamond, and graphite, have been investigated [14–20]. In an earlier molecular dynamics (MD) simulation focused on the collisions of a buckyball ( $C_{60}$ ) with a graphite (0001) surface, the energy dependence of the scattering properties in the impact energy region from

---

\*Corresponding author. Email: xqwang@gwu.edu

30 to 300 eV was studied. In this energy region, the  $C_{60}$  bounced back with its cage structure intact while snapshots showed that the graphite target evolved an inelastic and large deformation [15]. On the other hand, even though graphene is a building block of graphite, the mechanical properties of suspended graphene sheets deviate from the known properties of bulk graphite. Experiments have been undertaken to measure the effective spring constant of suspended graphene sheets (less than 5 layers) using an atomic force microscope (AFM) [21]. Experimental results show that the effective spring constant of graphene ranges from 1 to 5 N/m and the Young's modulus is 0.5 TPa, which is only about half of the Young's modulus of bulk graphite [21].

In this work, MD simulations were performed for the collisions between a buckyball and graphene. Although the basic motivation of this study was scientific curiosity, it may find some potential applications in offensive and defensive weapons (spear-shield) in future warfare. In the simulations, a square-shaped single-layer or double-layer graphene is simply supported along its two sides as the displacement-specified boundary conditions. A buckyball or a nano-onion approaches the center of the graphene perpendicularly with an impact velocity ranged from 4.37 km/s to 15.31 km/s. The choice to study the effect of impact velocity in this range is to demonstrate three distinctive phenomena: (i) buckyball bouncing back, (ii) buckyball and graphene sticking together, and (iii) buckyball penetrating through graphene. It should be mentioned that some researchers relate impact velocities with wavelength and natural frequency of vibration of buckyballs and graphene [22–24]. In all cases, ripples spread out from the collision point. The variations of the potential energy and the kinetic energy in time during the entire impact process are investigated.

## 2. Simulation model

In the MD simulations of collisions between buckyballs and graphene sheets, the square-shaped graphene is in the  $XY$  plane and the  $Z$  axis is normal to the graphene plane. The length (along the  $X$  axis) of the graphene layer is 11.11 nm, the width (along the  $Y$  axis) is 10.58 nm, and each layer contains 4549 atoms. The fixed displacement boundary condition applies to the carbon atoms within the bounds of 0.21 nm from the two edges parallel to the  $X$  axis. The buckyballs,  $C_{60}$  and  $C_{320}$ , are initially located above the center of the graphene at a sufficiently large distance so that there is no interaction between the buckyball atoms and the graphene atoms. Then a negative translational velocity component,  $V_z$ , is assumed to each atom of the buckyball or nano-onion. In this work, impact velocity refers to the magnitude of  $V_z$  and it varies from 4.37 km/s to 15.31 km/s (cf. Figure 1).

The empirical potential energy developed by Tersoff [25] is used to describe the interactions of the atoms in the system. The Tersoff potential accounts for the three-body interatomic forces and accurately describes the bonding in a wide range of carbon nanostructures. It is also deemed as one of the most advanced and sophisticated potential forms.

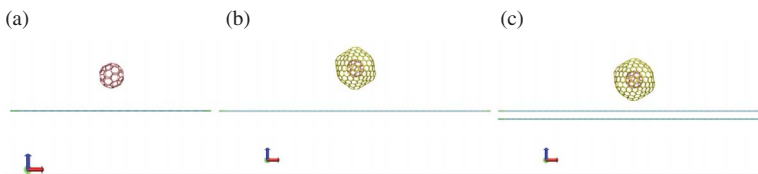


Figure 1. Configuration of the collision system: (a) buckyball ( $C_{60}$ ) and single-layer graphene; (b) nano-onion and single-layer graphene; (c) nano-onion and double2-layer graphene.

It gives the correct cohesive energy and the equilibrium lattice constant of graphene. In addition, researchers have showed that the Tersoff potential is stable in long-time running according to tests and gives fairly accurate results [26].

The total potential energy,  $E$ , in the Tersoff potential can be expressed as [25]:

$$E = \frac{1}{2} \sum_{i \neq j} V^{ij} = \frac{1}{2} \sum_{i \neq j} f_C(r^{ij}) \{f_A(r^{ij}) - b^{ij} f_B(r^{ij})\}, \quad (1)$$

where the two-body component and three-body component are:

$$f_C(r^{ij}) = \begin{cases} 1, & r^{ij} < D^{ij} \\ \frac{1}{2} \left\{ 1 + \cos \left[ \pi (r^{ij} - D^{ij}) / (S^{ij} - D^{ij}) \right] \right\}, & D^{ij} < r^{ij} < S^{ij} \\ 0, & r^{ij} > S^{ij} \end{cases} \quad (2)$$

$$f_A(r^{ij}) = A^{ij} \exp(-\lambda^{ij} r^{ij}), \quad (3)$$

$$f_B(r^{ij}) = B^{ij} \exp(-\mu^{ij} r^{ij}), \quad (4)$$

$$b^{ij} = [1 + \beta_i^{n_i} (\xi^{ij})^{n_i}]^{-1/2n_i}, \quad (5)$$

$$\xi^{ij} = \sum_{k \neq i,j} f_C(r^{jk}) g(\theta^{ijk}). \quad (6)$$

The more detailed expressions and material parameters are given in [25]. Accordingly, interatomic forces acting on all atoms involved in a potential component  $\frac{1}{2} V^{ij}$  can be obtained as:

$$\mathbf{F}^i = -\frac{1}{2} \{f'_C [f_A - b^{ij} f_B] + f_C [-\lambda^{ij} f_A + \mu^{ij} b^{ij} f_B]\} \frac{\mathbf{r}^{ij}}{r^{ij}} + \frac{1}{2} c^{ij} f_C(r^{ij}) f_B(r^{ij}) \frac{\partial \xi^{ij}}{\partial \mathbf{r}^i}, \quad (7)$$

$$\mathbf{F}^j = -\frac{1}{2} \{f'_C [f_A - b^{ij} f_B] + f_C [-\lambda^{ij} f_A + \mu^{ij} b^{ij} f_B]\} \frac{\mathbf{r}^{ij}}{r^{ij}} + \frac{1}{2} c^{ij} f_C(r^{ij}) f_B(r^{ij}) \frac{\partial \xi^{ij}}{\partial \mathbf{r}^j}, \quad (8)$$

$$\mathbf{F}^k = \frac{1}{2} c^{ij} f_C(r^{ij}) f_B(r^{ij}) \frac{\partial \xi^{ij}}{\partial \mathbf{r}^k}, \quad (9)$$

where

$$\frac{\partial \xi^{ij}}{\partial \mathbf{r}^i} = \left\{ g f'_C(r^{ik}) \frac{\mathbf{r}^{ik}}{r^{ik}} + d^{ij} \frac{\partial \cos \theta^{ijk}}{\partial \mathbf{r}^i} \right\}, \quad (10)$$

$$\frac{\partial \xi^{ij}}{\partial \mathbf{r}^j} = d^{ij} \frac{\partial \cos \theta^{ijk}}{\partial \mathbf{r}^j}, \quad (11)$$

$$\frac{\partial \xi^{ij}}{\partial \mathbf{r}^k} = \left\{ -g f'_C(r^{ik}) \frac{\mathbf{r}^{ik}}{r^{ik}} + d^{ij} \frac{\partial \cos \theta^{ijk}}{\partial \mathbf{r}^k} \right\}, \quad (12)$$

$$c^{ij} \equiv -0.5\beta_i (\beta_i \xi^{ij})^{n_i-1} [1 + (\beta_i \xi^{ij})^{n_i}]^{-1/2n_i-1} \quad (13)$$

$$d^{ij} \equiv f_C(r^{ik}) \frac{-2c_i^2 (h_i - \cos \theta^{ijk})}{[d_i^2 + (h_i - \cos \theta^{ijk})^2]^2} \quad (14)$$

$$\frac{\partial \cos \theta_{ijk}}{\partial \mathbf{r}^i} = \left( \frac{1}{r^{ik}} - \frac{\cos \theta_{ijk}}{r^{ij}} \right) \frac{\mathbf{r}^{ij}}{r^{ij}} + \left( \frac{1}{r^{ij}} - \frac{\cos \theta_{ijk}}{r^{ik}} \right) \frac{\mathbf{r}^{ik}}{r^{ik}} \quad (15.1)$$

$$\frac{\partial \cos \theta_{ijk}}{\partial \mathbf{r}^j} = \frac{\cos \theta_{ijk}}{r^{ij}} \frac{\mathbf{r}^{ij}}{r^{ij}} - \frac{1}{r^{ij}} \frac{\mathbf{r}^{ik}}{r^{ik}} \quad (15.2)$$

$$\frac{\partial \cos \theta_{ijk}}{\partial \mathbf{r}^k} = \frac{\cos \theta_{ijk}}{r^{ik}} \frac{\mathbf{r}^{ik}}{r^{ik}} - \frac{1}{r^{ik}} \frac{\mathbf{r}^{ij}}{r^{ij}} \quad (15.3)$$

The equations of motion governing the dynamics of the system are solved by the velocity Verlet algorithm. In the simulations, a typical time step was 0.24 fs. The codes were developed by researchers at the George Washington University.

### 3. Results and discussion

Figure 2 confirms that total energy, the sum of kinetic energy and potential energy, is conserved since there is no dissipation in a classical MD simulation. For the  $i$ th atom, we have the governing equation

$$m^i \dot{\mathbf{v}}^i = \mathbf{F}^i \quad (16)$$

and the interatomic ‘constitutive relationship’

$$\mathbf{F}^i = -\frac{\partial E_p}{\partial \mathbf{r}^i}. \quad (17)$$

Since, the time dependence of the kinetic energy and potential energy are

$$\frac{dE_k}{dt} = \frac{d}{dt} \left( \sum_i \frac{1}{2} m^i v^{i2} \right) = \sum_i m^i \dot{\mathbf{v}}^i \mathbf{v}^i \quad (18.1)$$

$$\frac{dE_p}{dt} = \sum_i \frac{\partial E_p}{\partial \mathbf{r}^i} \dot{\mathbf{r}}^i = -\sum_i \mathbf{F}^i \mathbf{v}^i \quad (18.2)$$

from Equation (16) it is easy to obtain

$$\sum_i m \dot{\mathbf{v}}^i \mathbf{v}^i = \sum_i \mathbf{F}^i \mathbf{v}^i. \quad (19)$$

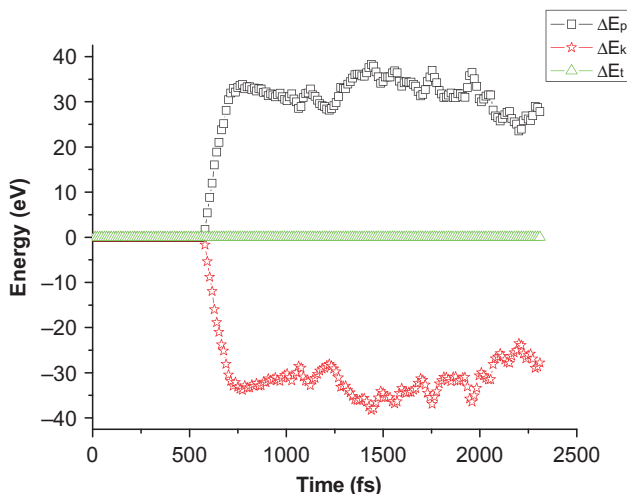


Figure 2. Time evolution of energy changes from their initial values for the  $C_{60}$ -graphene collision as shown in Figure 3a (impact velocity 4.37 km/s). The diamond symbol designates the potential energy change of the whole system,  $\Delta E_p$ . The star symbol denotes the kinetic energy change of the whole system,  $\Delta E_k$ . The triangle symbol gives the total energy change of collision system,  $\Delta E_t$ .

Combining Equations (18) and (19), one can draw the following conclusion that the sum of kinetic and potential energies is conserved:

$$\frac{dE_k}{dt} + \frac{dE_p}{dt} = \frac{d(E_k + E_p)}{dt} = 0. \quad (20)$$

In this case, conservation of energy is confirmed by numerical results. This result provides confidence for the MD simulation of carbon nanostructures based on the Tersoff potential. The simulation result also confirms that the greatest potential is obtained at the moment of largest deformation.

The simulation results for a collision between a buckyball ( $C_{60}$ ) and single-layer graphene are shown in Figure 3. When the impact velocity of  $C_{60}$  is relatively small (less than 8.75 km/s), the buckyball bounces back (Figure 3a) and the collision generates ripples spreading out from the contact region on the graphene plane. As the impact velocity increases, roughly ranging from 8.75 km/s to 12.03 km/s, the buckyball sticks to the graphene. The buckyball is broken when the impact velocity is larger than 12.03 km/s. But no matter how large the impact velocity is, the buckyball cannot go through the graphene layer without suffering obvious damage.

For a nano-onion and single-layer graphene collision, the phenomena of bouncing back and sticking together are observed when the impact velocity is less than 9.84 km/s. When the graphene layer is broken, there are two possibilities for the nano-onion. If the impact velocity is very large, say, greater than 14.22 km/s, both the outer and inner buckyballs are broken. The reason is that the outer one deforms severely and generates a huge force on the inner one. On the other hand, if the impact velocity is not so large, say, 10.93 km/s, even though the outer one is broken, the inner one penetrates the graphene layer intact, as shown as Figure 4. The outer layer of the nano-onion becomes a protector of its inner structure. When the single-layer graphene is replaced by a double-layer graphene, the results

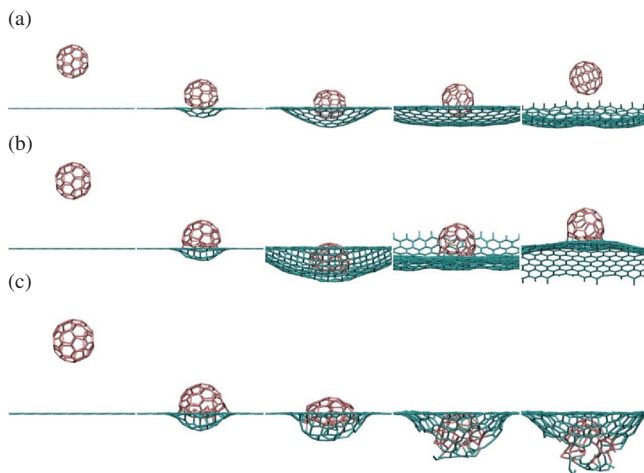


Figure 3. Snapshots of collisions between a buckyball and single-layer graphene with different initial impact velocities: (a) 4.37 km/s; (b) 10.93 km/s; (c) 13.13 km/s.

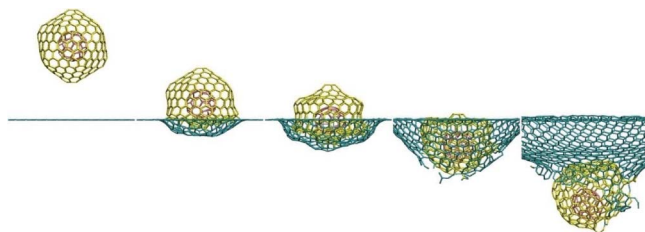


Figure 4. Snapshots of collision between nano-onion with initial impact velocity 10.93 km/s and single-layer graphene.

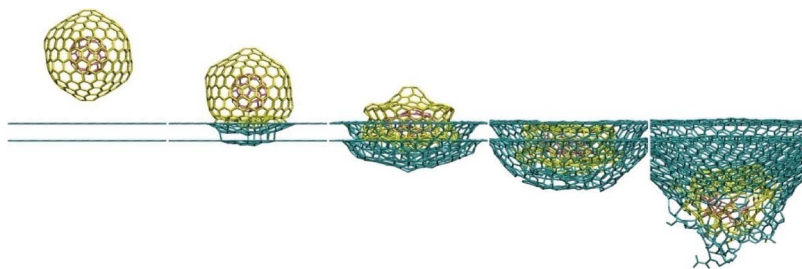


Figure 5. Snapshots of collision between nano-onion with initial impact velocity 13.13 km/s and double-layer graphene.

are similar, except that the inner buckyball cannot stay intact after collision, as shown in Figure 5.

The deformation factor  $\alpha$  [14], which is defined as the ratio  $\alpha \equiv r_z/r_{xy}$ , is used to describe the deformation of  $C_{60}$ . Here  $r_{xy}$  and  $r_z$  are the maximal and minimal radii of the ellipsoid-like molecule, respectively. Compared with the result for a  $C_{60}$ -graphite collision [14], the molecule experiences large deformation twice, rather than once, at  $t = 640$  fs and  $t = 770$  fs. At  $t = 640$  fs, the bottom of the  $C_{60}$  molecule just arrives on the graphene

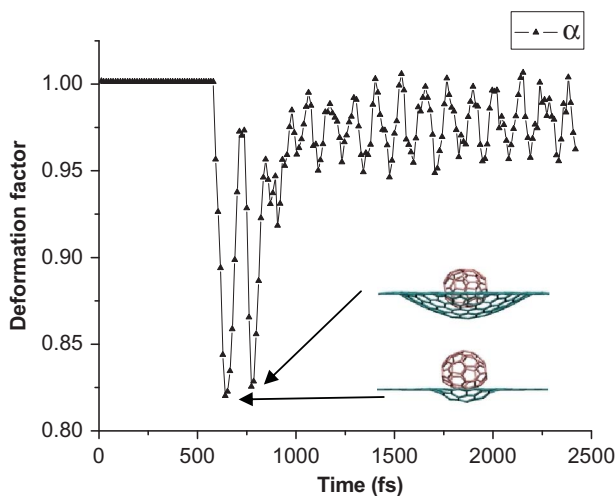


Figure 6. The deformation factor  $\alpha$  changes with time for the buckyball–graphene collision as shown in Figure 3a.

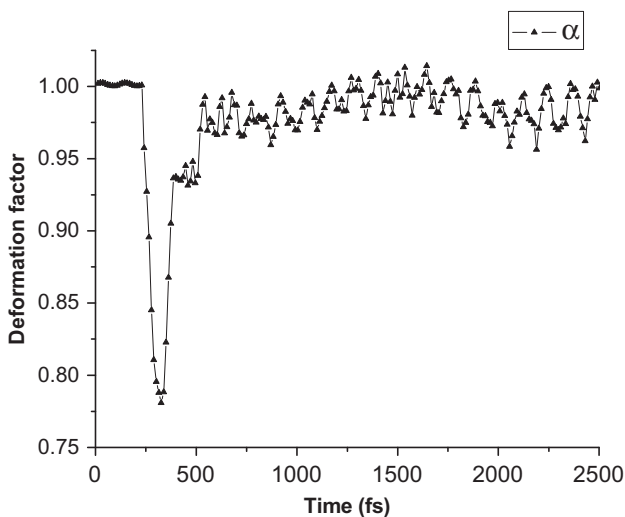


Figure 7. The potential energy of the buckyball changes with time for the  $C_{60}$ –graphene collision shown in Figure 3a.

plane and receives its maximal deformation (cf. Figure 6) and largest potential energy (cf. Figure 7). But along the  $Z$ -axis, the center of mass velocity is not zero. As it moves on, the molecule falls onto the graphene surface. The dented graphene pushes the deformed buckyball to regain its sphere-like shape, which leads to a increase of the deformation factor before the buckyball rebounds. The buckyball gains its minimal kinetic energy and second largest potential energy at  $t = 770$  fs. Then the buckyball begins to bounce back from the graphene and regains its sphere-like shape again.

Deformation factor evolution for a collision between a buckyball at the same impact velocity as the collision event in Figure 3a with an eight-layer graphene was carried out



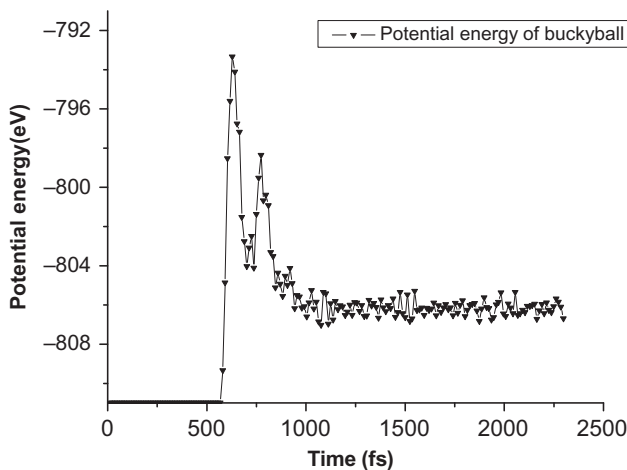


Figure 8. The deformation factor  $\alpha$  changes with time for the collision between a buckyball and an eight-layer graphene with impact velocity 4.37 km/s, i.e. the same impact velocity as in Figure 3a. The potential energy of buckyball changes with time for the  $C_{60}$ -graphene collision as shown in Figure 3a.

as a comparison, as shown as Figure 8. The largest deformation factor is higher than that of the collision in Figure 3a, while the second largest deformation factor becomes smaller. As a general rule, as the number of graphene layers increases, the characteristics of the buckyball being deformed severely and then regaining its sphere-like shape twice becomes inconspicuous. As for graphite, this kind of characteristics disappears, as in Figure 2 in [7].

#### 4. Conclusion

The collisions between buckyballs and graphene sheets were investigated based on MD simulations with impact velocity ranging from 4.37 km/s to 15.31 km/s. The buckyball and nano-onion will bounce back at low energies, stick together at higher energies, and break up at very high collision energies. For a nano-onion, the outer structure will become a protector when the impact velocity is within a proper range. From Figures 2-4, it can be seen that the nanostructures of both buckyball and graphene undergo extraordinary large deformations during collisions. The incident  $C_{60}$  experiences the process of deforming severely and then regaining its sphere-like shape twice. These simulation results demonstrate that the impact velocity plays a crucial role in collisions between carbon nanostructures. The results may provide some useful clues for applications of graphene involving sudden directional compression.

#### References

- [1] A.K. Geim, *Graphene: Status and prospects*, Science 324 (2009), pp. 1530–1534.
- [2] C. Lee, X. Wei, J.W. Kysar, and J. Hone, *Measurement of the elastic properties and intrinsic strength of monolayer graphene*, Science 321 (2008), pp. 385–388.
- [3] A.K. Geim and K.S. Novoselov, *The rise of graphene*, Nat. Mater. 6 (2007), pp. 186–191.
- [4] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos, and A.A. Firsov, *Two-dimensional gas of massless Dirac fermions in graphene*, Nature 438 (2005), pp. 197–200.

- [5] S.V. Morozov, K.S. Novoselov, M.I. Katsnelso, F. Schedin, D.C. Elias, J.A. Jaszczak, and A.K. Geim, *Giant intrinsic carrier mobilities in graphene and its bilayer*, Phys. Rev. Lett. 100 (2008), 016602.
- [6] U. K ur um, O. . Ekiz, H.G. Yaglioglu, A. Elmali, M.  rel, H. G uner, A.K. Mızrak, B. Ortaç, and A. D ana, *Electrochemically tunable ultrafast optical response of graphene oxide*, Appl. Phys. Lett. 98 (2011), 141103.
- [7] J. Liu, A.R. Wright, C. Zhang, and Z. Ma, *Strong terahertz conductance of graphene nanoribbons under a magnetic field*, Appl. Phys. Lett. 93 (2008), 041106.
- [8] K. Saito, J. Nakamura, and A. Natori, *Ballistic thermal conductance of a graphene sheet*, Phys. Rev. B 76 (2007), 115409.
- [9] A.A. Balandin, S. Ghosh, W. Bao, I. Calizo, D. Teweldebrhan, F. Miao, and C.N. Lau, *Superior thermal conductor graphene*, Nano Lett. 8 (2008), pp. 902–907.
- [10] J.S. Bunch, A.M. Van Der Zande, S.S. Verbridge, I.W. Frank, D.M. Tanenbaum, J.M. Parpia, H.G. Craighead, and P.L. McEuen, *Electromechanical resonators from graphene sheets*, Science 315 (2007), pp. 490–493.
- [11] L.A. Ponomarenko, F. Schedin, M.I. Katsnelson, R. Yang, E.W. Hill, K.S. Novoselov, and A.K. Geim, *Chaotic Dirac billiard in graphene quantum dots*, Science 320 (2008), pp. 356–358.
- [12] N. Mohanty and B. Vikas, *Graphene-based single-bacterium resolution biodevice and DNA-transistor: Interfacing graphene-derivatives with nanoscale and microscale biocomponents*, Nano Lett. 8 (2008), pp. 4469–4476.
- [13] J. Lu, P.E. Yeo, C.K. Gan, P. Wu, and K.P. Loh, *Transforming C<sub>60</sub> molecules into graphene quantum dots*, Nat. Nanotech. 6 (2011), pp. 247–252.
- [14] Z.Y. Man, Z.Y. Pan, and Y.K. Ho, *The rebounding of C<sub>60</sub> on graphite surface: A molecular dynamics simulation*, Phys. Lett. A 209 (1995), pp. 53–56.
- [15] Z.Y. Pan, Z.Y. Man, Y.K. Ho, J. Xie, and Y. Yue, *Energy dependence of C<sub>60</sub>–graphite surface collisions*, J. Appl. Phys. 83 (1998), pp. 4963–4967.
- [16] R.D. Beck, P.S. John, M.M. Alvarez, F. Diederich, and R.L. Whetten, *Resilience of all-carbon molecules C<sub>60</sub>, C<sub>70</sub>, and C<sub>84</sub>: A surface-scattering time-of-flight investigation*, J. Phys. Chem. 95 (1991), pp. 8402–8409.
- [17] R.C. Mowrey, D.W. Brenner, B.I. Dunlap, J.W. Mintmire, and C.T. White, *Simulations of buckminsterfullerene (C<sub>60</sub>) collisions with a hydrogen-terminated diamond {111} surface*, J. Phys. Chem. 95 (1991), pp. 7138–7142.
- [18] R. Smith and R.P. Webb, *Energetic fullerene interactions with a graphite surface*, Proc. Roy. Soc. Lond.: Math. Phys. Sci. 441 (1993), pp. 495–499.
- [19] H.G. Busmann, T. Lill, and I.V. Hertel, *Near specular reflection of C<sub>60</sub> ions in collisions with an HOPG graphite surface*, Chem. Phys. Lett. 187 (1991), pp. 459–465.
- [20] Z.Y. Pan, Z.Y. Man, and M. Hou., *Z. Phys. D 41 (1997)*, pp. 275–280.
- [21] I.W. Frank, D.M. Tanenbaum, A.M. van der Zande, and P.L. McEuen, *Mechanical property of suspended graphene sheets*, J. Vac. Sci. Tech. B 25 (2007), pp. 2558–2561.
- [22] Y. Chandra, R. Chowdhury, F. Scarpa, and S. Adhikari, *Vibrational characteristics of bilayer graphene sheets*, Thin Solid Film 519 (2011), pp. 6026–6032.
- [23] S. Adhikari and R. Chowdhury, *Vibration spectra of fullerene family*, Phys. Lett. A 375 (2011), pp. 1276–1280.
- [24] R. Chowdhury, S. Adhikari, F. Scarpa, and M.I. Friswell, *Transverse vibration of single layer graphene sheets*, J. Phys. D: Appl. Phys. 44 (2011), 205401.
- [25] J. Tersoff, *Modeling solid-state chemistry: Interatomic potentials for multicomponent systems*, Phys. Rev. B 39 (1989), pp. 5566–5568.
- [26] Z. Yao, J. Wang, B. Li, and G. Liu, *Thermal conduction of carbon nanotubes using molecular dynamics*, Phys. Rev. B 71 (2005), 085417.