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Impact dynamics of graphene nanosheets in collision with metallic nanoparticles

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Tangential coefficient of restitution;
Collision.

Abstract. In this paper, impact of metallic nanoparticles on graphene sheets was investigated via Non-Equilibrium Molecular Dynamics (NEMD) approach. Considering the unique feature of graphene to absorb motion energy of the materials impacting on it, systems based on graphene can be appropriate solutions for the purpose of damping. The proposed model was validated by available experimental data and simulation. It is demonstrated that mechanics of impact are not multidimensional problems; therefore, they can be studied by molecular dynamics. Effects of velocity of the particles, impact angle, and number of the graphene sheets on the normal coefficient of restitution of the metallic nanoparticles were researched. Contrarily to macro systems, it was observed that by increasing the velocity of impact, normal coefficient of restitution decreased. Also, the normal coefficient of restitution increased by increasing impact angle. By increasing the graphene sheets, the coefficient was reduced significantly. Negative normal coefficient of restitution was observed for some cases, which was also reported in other works on nanostructures. It is shown that a single graphene layer can withstand impacting 3.64 times a 20-layer graphene sheet.

1. Introduction

Collision of two or several particles is one of the most fundamental problems in physics, chemistry, and engineering. In the evolution of impact theory, four major aspects emerged as distinct (but not unrelated) subjects of interest. Depending on the impact characteristics (i.e., velocity, materials), supposed assumptions, and achieved results, one aspect will become more predominant, leading to a solution approach for impact analysis. These four aspects are classical mechanics, elastic stress wave propagation, contact mechanics, and plastic deformation. Classical mechanics involves the application of fundamental laws of mechanics to predict the velocities after impact. The impulse-momentum law forms the core of this approach. Brach uses this approach exclusively in [1] to model numerous practical problems. The algebraic nature of this method makes the mathematical development easy and accessible to most engineers. The loss of energy inherent in any real impact process is taken into account by means of the normal coefficient of restitution. The accuracy of this coefficient is crucial to obtain acceptable results.

As an amazing technology-based material with a great potential in impact problems, graphene, the atomic single- and few-layer carbons in a honey comb configuration, has been discovered in the recent decade. Graphene has a high-strain-rate behavior over a range of thicknesses from 10 to 100 nanometers (equivalent to 30 to 300 graphene layers) based on ballistic tests [2]. In this experiment, tensile stretching of the membrane into a cone shape was followed by initiation of radial cracks, which approximately followed crystallographic

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directions and extended outward well beyond the impact area. Energy per unit mass needed for penetration of projectiles is defined as specific penetration energy. The specific penetration energy for Few-Layer Graphene Sheets (FLGS) was reported ∼10 times the literature values for macroscopic steel sheets for impact velocity of 600 meters per second [2]. As a common impact study, Avila et al. focused on ballistic tests of hybrid nanocomposites. The two hybrid nanocomposites studied were fiber glass/epoxy/nanoclay and fiber glass/epoxy/nanographite [3]. To understand behavior of the material in irradiative environment, ion implantation and irradiation of graphene by using the ion bombardment process were investigated and it was found that larger incident angles were desired for substitution and single vacancies, whereas smaller incident angles were favored for forming double vacancies, multiple vacancies, and in-plane disorder [4]. The bombardment of a suspended monolayer graphene sheet via different energetic atoms via classical molecular dynamics based on the reactive force field (ReaxFF) was studied [5]. It was found that the probability, quality, and controllability of defects were mainly determined by the impact site, the properties of the incident atom, and the incident energy. By combining ion beam experiments and atomistic simulations, the production of defects in graphene on Ir(111) under grazing incidence of low-energy Xe ions was also studied [6]. It was demonstrated that the ions were channeled between graphene and the substrate, giving rise to chains of vacancy clusters with their edges bending down toward the substrate.

As a basic concept of the classical mechanics, normal coefficient of restitution was introduced long ago by Newton. This coefficient addresses impact of macroscopic bodies. According to a standard definition, it is equal to the ratio of the normal component of the rebound speed V_2 to the impact speed V_1 as $RC = V_2/V_1$ when the secondary object is fixed. Recently, researchers explained the coefficient of restitution of objects impacting on graphene layers [7]. They developed a theory of an oblique impact, based on continuum model of particles, and a good agreement between the macroscopic theory and simulations was observed. This led to the validity of macroscopic concepts of elasticity, bulk viscosity, and surface tension for nanoclusters including a few hundred atoms [7,8].

Some studies investigated collision of clusters with graphene sheets [7-10]. By using the molecular dynamics simulations, they generally investigated the collision of a few argon atoms on the graphene (single-layer) sheets.

This paper develops previous works to have a valuable view on the effect of number of layers and also collision of various clusters on the graphene sheets. Furthermore, collision of metallic nanoparticles on the graphene sheets is considered. Multi-scale approaches are essential to predict correct dynamics of both small and large scales in mixed-scale systems such as graphene-based nanoresonators and sensors. In this paper, a multiscale approach is used to show that restitution coefficient is not significantly size-dependent; in the conclusion, it is shown that the results of the applied molecular dynamic simulation are valid.

2. Theory

Figure 1 shows the general configuration of a nanoparticle thrown onto a graphene nanosheet. Generally, polymer base should be considered in dynamics of the system, but, in order to focus on the effects of graphene layers on the coefficient of restitution, it is assumed that only graphene layers are placed at the substrate as an obstacle.

Nanoparticle was thrown onto the graphene sheet and, then, the nanoparticle deformed and lied on the sheet. The greatest portion of energy transfer occurred at this step. Then, due to restitutional nature of the collision, the nanoparticle returned from the surface of nanosheet. A considerable deformation of nanoparticle could be observed after leaving the graphene nanosheet.

By using the LAMMPS package, MD (Molecular Dynamics), the discrete equations of motion are derived as:

$$m_i \ddot{u}_i = -\nabla_i U(u_1 : u_N), \tag{1}$$

where, m_i, u_i, and $U(u_1 : u_N)$ are mass, displacements, and interatomic potentials for N atoms, respectively. Tersoff potential [11] was used for interaction of carbon atoms and pair coefficients that were chosen from [11]. As interfacial force field (graphene-graphene and graphene-metals), a Lennard-Jones potential was differentiated with the coefficients listed in Table 1. Values of depth of the potential well (ε (eV)) and

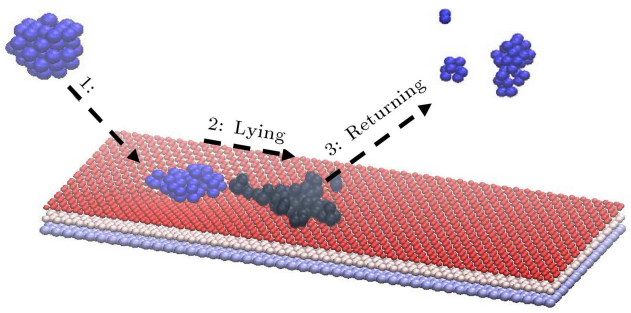

Figure 1. General configuration of a nanoparticle thrown onto a graphene nanosheet; 1: Throwing the nanoparticle onto the graphene sheet; 2: Lying the nanoparticle on the graphene sheet via deformation; 3: Rturning from graphene nanosheet after discharging a few parts of kinetic energy.

Table 1. Lennard-Jones parameters for simulated metals and carbon.

Material	Lattice structure [21]	Lattice constant, r (A)	Molar mass, m (g/mol)	σ (A) [21]	ε (eV) [21]
Ag	FCC	4.085	107.8682	2.955	0.19608
Al	FCC	4.0496	26.98	2.925	0.17286
Au	FCC	4.080	196.97	2.951	0.22747
Cu	FCC	3.610	63.54	2.616	0.20296
Ni	FCC	3.520	58.69	2.552	0.24295
Pd	FCC	3.890	106.42	2.819	0.26445
Pt	FCC	3.924	195.09	2.845	0.33540
C	Honeycomb	3.37	12.011	3.41	0.00239

the finite distance, at which the inter-particle potential was zero ($\sigma(\mathring{A})$), were obtained from Lorentz-Berthelot mixing rules: ($\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}$) and $\sigma_{ij} = \frac{1}{2}(\sigma_{ii} + \sigma_{jj})$. For carbon atoms, $\varepsilon = 0.00239$ eV and $\sigma = 3.41$ A. In the whole simulation, fixing two rows of carbon atoms on all edges was used as the boundary condition [12].

When a nanocluster impacts on the graphene sheet with a given velocity, the momentum equation ($m_{\text{cluster}}v_{\text{cluster}}+m_{GF}v_{GF} = m_{\text{cluster}}v'_{\text{cluster}}+m_{GF}v'_{GF}$) contains two unknowns (v'_{cluster} and v'_{GF}) and we clearly need an additional relationship to find the final velocities. Reflecting the capacity of the contacting bodies to recover from the impact, normal coefficient of restitution (e) is defined as the ratio of magnitude of the restoration impulse to the magnitude of the deformation impulse. It helps us to use an additional relationship. As shown in Figure 2, let F_r and F_d represent the magnitudes of the contact forces during the restoration and deformation periods, respectively.

Then, for the nanocluster, the definition of 'e', together with the impulse momentum equation, gives:

$$e = \frac{\int_{t_0}^{t_1} F_r dt}{\int_0^{t_0} F_d dt} = \frac{m_{NC}\left[-v'_{NC} - (-v_0)\right]}{m_{NC}\left[-v_0 - (-v_{NC})\right]} = \frac{v_0 - v'_{NC}}{v_{NC} - v_0}. \quad (2)$$

Similarly, for the graphene layer, we have:

$$e = \frac{\int_{t_0}^{t_1} F_r dt}{\int_0^{t_0} F_d dt} = \frac{m_G\left[v'_G - v_0\right]}{m_G\left[v_0 - v_G\right]} = \frac{v'_G - v_0}{v_0 - v_G}. \quad (3)$$

Then, by eliminating v_0 between the two expressions for 'e', we would have:

$$e = \frac{v'_G - v'_{NC}}{v_{NC} - v_G} = \frac{|\text{Relative velocity of separation}|}{|\text{Relative velocity of approach}|}. \quad (4)$$

If the two initial velocities, v_{NC} and v_G, and the normal coefficient of restitution 'e' are known, then impact problem is completely predictable.

It should be noted that normal coefficient of restitution must be associated with a pair of contacting bodies. The normal coefficient of restitution is frequently considered as a constant for given geometries and a given combination of contacting materials [13]. Actually, it depends on the impact velocity and approaches unity as the impact velocity approaches zero with increasing relative impact velocity [14]. However, such behavior is not valid in the case of collision of nanoparticles with graphene sheets. This will be discussed in the following sections. For collision

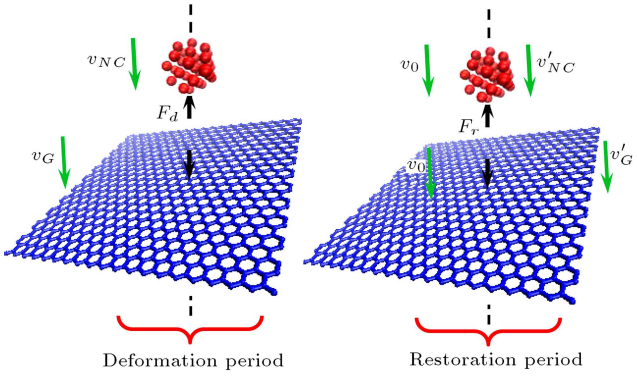

Figure 2. Deformation and restoration periods for impacting a nanocluster on a graphene sheet.

between large bodies, a handbook value for 'e' is generally unreliable; thus, in the case of nanometric geometries, such values are unreliable and, for each problem, an appropriate table to find the correct value should be derived. Although experiments are more valuable, there is still no possible test procedure for small scales. Therefore, validated simulations can be helpful to introduce some design tables and diagrams.

By having constant impact velocity, it is possible to reduce the rebound velocity of nanoparticles in manufacturing processes. This can be used for trapping nanoparticles on the layered graphene sheets. This is the main idea for gas storage. Bombardment of graphene sheets by several gaseous molecules [15] and especially oxygen [4] was studied to control defect generation [16]. Furthermore, some recent works focused on mass detection of metallic nanoparticles [17]. In this paper, after some validation studies, normal and tangential coefficients of restitution are calculated for collision of metallic nanoparticles with single- and few-layer graphene sheets.

3. Validation

3.1. Comparison of specific penetration energies

The specific energy dissipation, $E_p^* = E_p(\rho A_s h_{\text{ave}})^{-1}$, which is insensitive to material density, by taking account of the mass within $\rho A_s h_{\text{ave}}$, is given by $E_p^* = \frac{V_{\text{impact}}^2}{2} + E_d^*$, where E_d^* is the specific delocalized penetration energy [2]. Figure 3 depicts the specific penetration energy for SLG (single-layer graphene) to 20-layer graphene sheets and also steel, aluminum, and gold plates under a steel nano-bullet with various impact velocities. Since the projectile size and weight are very smaller than those mentioned in [2], the required critical velocity for thrusting the plates is very higher. Figure 3 shows that graphene-based plate has a considerably higher resistance against the projectile than metal micro plates.

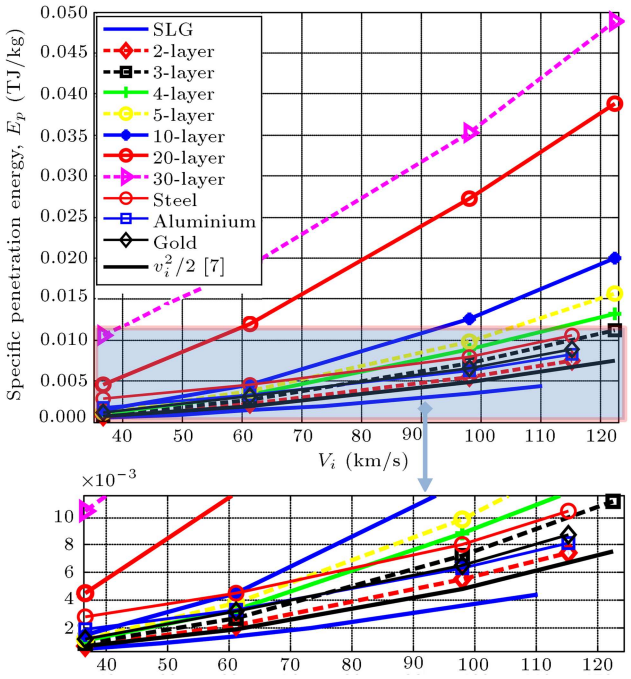

Figure 3. Specific penetration energy versus impact velocity for various materials.

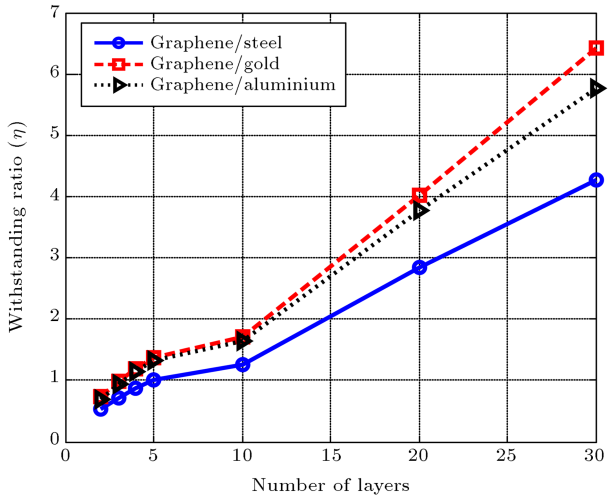

Figure 4. Withstanding ratio of graphene in comparison to those of the steel, gold, and aluminum plates for various FLGs.

By averaging the specific penetration energies along various velocities, Figure 4 shows the withstanding ratio of few-layer graphene sheets in comparison with the steel, gold, and aluminum plates. The formula for five-layer sheets is as follows:

$$\eta_{G-St} = \frac{\sum_{V_{i1}}^{V_{i4}} E_{p_{\text{Graphene}}}^*}{\sum_{V_{i1}}^{V_{i4}} E_{p_{\text{Steel}}}^*}. \tag{5}$$

3.2. Comparison of graphene's deflection

Figure 5 shows the comparison of simulation results of the mean deflection of the graphene, which are averaged over the azimuthal coordinate at 2.2 and 2.8 ps. The incident cluster contained 500 argon atoms and the incident speed was 316 m/s. The magnitude of the impulse was 1.96×10^{-22} N.s. It was also observed that for higher velocities, the argon cluster exploded; therefore, comparison was not possible as it is reported in [7].

4. Results and discussion

Normal and tangential coefficients of restitution ('e' and RC_x) for some metals have been studied. Silver, gold, aluminum, copper, nickel, palladium, and platinum were simulated in a collision process in which graphene sheets were considered as a barrier and were

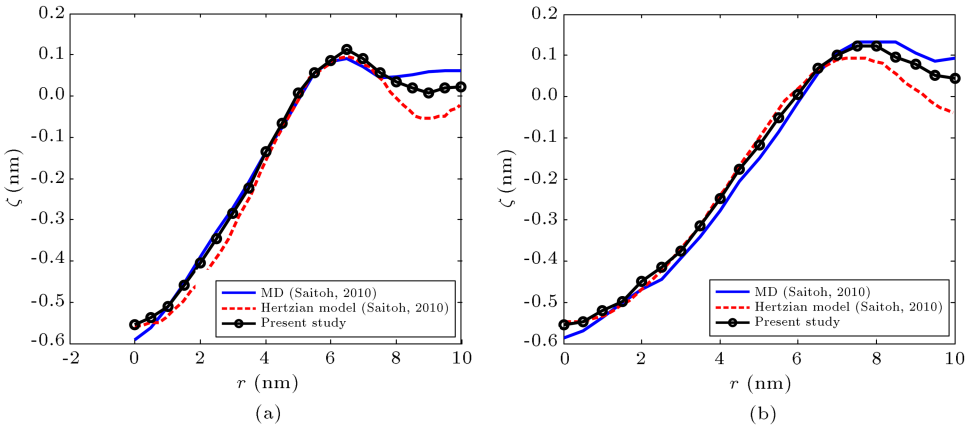

Figure 5. Comparison of simulation results of the mean deflection of the graphene, which are averaged over the azimuthal coordinate, and those of the previous work at (a) 2.2 ps and (b) 2.8 ps.

assumed to be fixed on all boundaries before and after cluster impact. This guarantees simple calculation of the normal coefficient of restitution by eliminating the effect of momentum of the system on the impact time.

4.1. Effects of impact velocity

Figure 6 depicts the deflection of a 3 × 9 nm SLG and deformation of a gold nanocluster in an oblique collision with the layer. Rebound from xz plane on the middle line of SLG is observable.

Figure 7 shows the normal and tangential coefficients of restitution (e and RC_x) for gold nanoparticles versus various impact velocities. Tangential coefficient of restitution was calculated by:

$$RC_x = \frac{v'_{G_x} - v'_{NC_x}}{v_{NC_x} - v_{G_x}} = \frac{|\text{Relative velocity of landing}|}{|\text{Relative velocity of rebounding}|}. \quad (6)$$

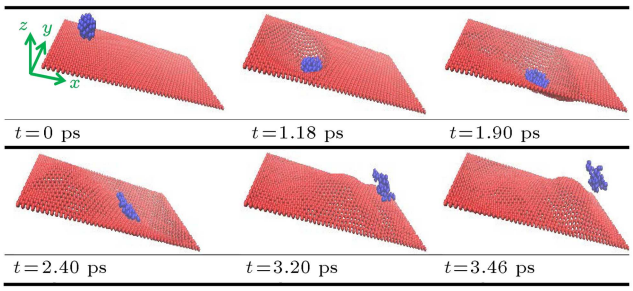

Figure 6. Deflection of a 3 × 9 nm SLG and deformation of gold nanoparticle in an oblique collision with the single graphene layer.

Figure 7 also contains the multi-scale responses for 6 × 6 nm SLG (on the middle of a 90 × 90 μm^2 plate).

The used multi-scale method was based on [18-20] and it was fitted to current metallic nanoparticles impact on graphene sheets problem. Because of low stress induction on graphene sheets, low impact duration, and low wavelength of impact, this problem is not multi-scale; thus, it can be investigated only by NEMD. Comparisons are shown in Figure 7. As can be seen, the multi-scale results are not significantly different from Non Equilibrium Molecular Dynamics (NEMD) for various sheets.

Increasing horizontal impact velocity decreases the tangential coefficient of restitution, whereas the

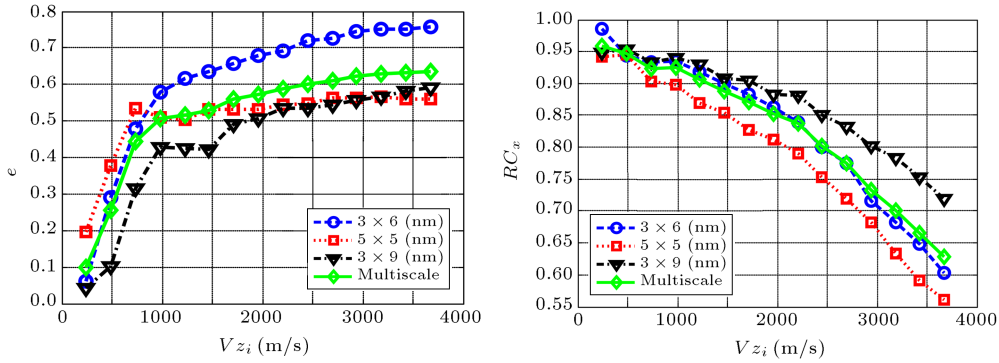

Figure 7. Normal and tangential coefficients of restitution (e and RC_x) for collision of gold nanoparticle with SLGS with various dimensions.

normal coefficient of restitution increases with increasing impact velocity. This is due to the momentum-related resistance of SLG against the faster impacted projectile. As discussed earlier, for macro bodies, the normal coefficient of restitution depends on the impact velocity and decreases when relative impact velocity increases [14]. Figure 7 shows that such behavior is not valid in the case of collision of nanoparticles with graphene sheets.

4.2. Effects of impact angle

When a nanocluster impacts on the graphene surface, some new options will be expected. To address the dependency of normal coefficient of restitution on the impact angle, an especial operation has been simulated here. Nanoclusters were thrown onto a specific point (0,0,0) of an SLG along the $x-z$ plane with various angles θ_i like those depicted in Figure 8.

Same as what is demonstrated in Figure 8, metallic nanoparticles were thrown onto an SLG with several impact angles. Figure 9 shows the effect of impact angle on the normal coefficient of restitution between metallic nanoparticles and single-layer graphene sheet. It was clearly observed that almost all particles had the same behavior with close scaling amplitudes in normal coefficient of restitution. However, the calculated normal coefficient of restitution for aluminum was approximately constant, whereas for other materials, it thoroughly followed the fitted quadratic equation as $e(\theta) = 0.418\theta^2 - 0.045\theta - 0.396$, where θ is in radian. This equation was obtained by averaging the coefficients of restitution along impact angle. It should be noted that since responses in the case of angles greater than $\theta = 80°$, due to the edge effects, diverged, they are neglected in the figures.

Figure 10 depicts the tangential coefficient of

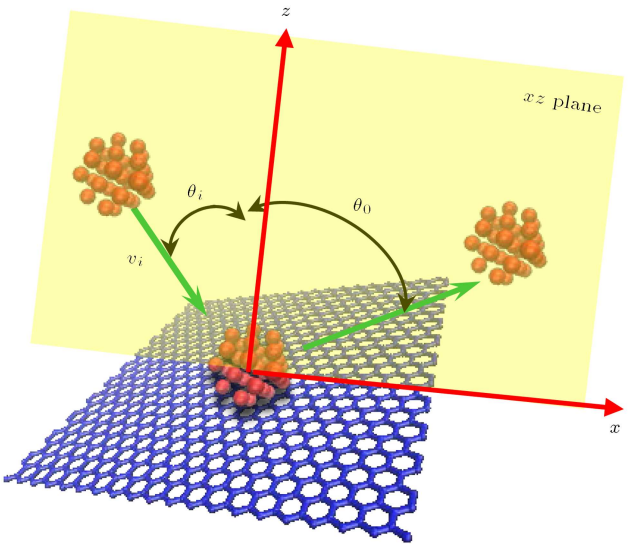

Figure 8. An especial operation to depict dependency of rebound behavior on the impact angle.

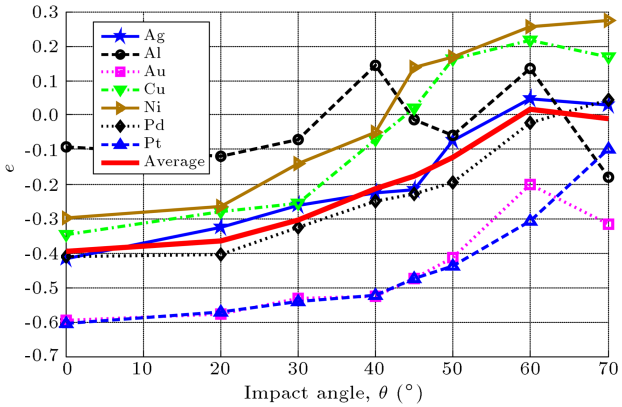

Figure 9. Normal coefficient of restitution for various metallic nanoparticles thrown onto an SLG with various impact angles.

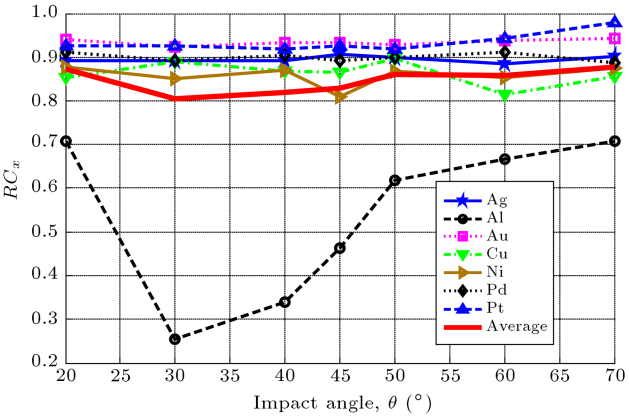

Figure 10. Tangential coefficient of restitution for various metallic nanoparticles thrown onto an SLG with various impact angles.

restitution for various impact angles. Although aluminum behaved completely different here, other materials followed the average diagram that is approximately a cubic relation as $RC_x(\theta) = -0.9121\theta^3 + 2.371\theta^2 - 1.857\theta + 1.267$, where θ is in radian.

4.3. Effects of number of layers of graphene sheets

Figure 11 shows the deformation of graphene plates under firing with nano-metallic particles. Due to dropping of the particles with the same initial velocity (by applying an external force proportional to the mass on the first 500 time steps of integration), all the particles collided with the plates at $t = 70$ fs, but left the plate at various times. For various numbers of layers, particles had different positions and shapes at $t = 175$ fs and later on.

As Figure 12 shows, increasing the number of layers decreased the normal coefficient of restitution. All simulations were performed with $\theta = 30°$. Normal coefficients of restitution for gold and platinum particles, which had approximately the same values,

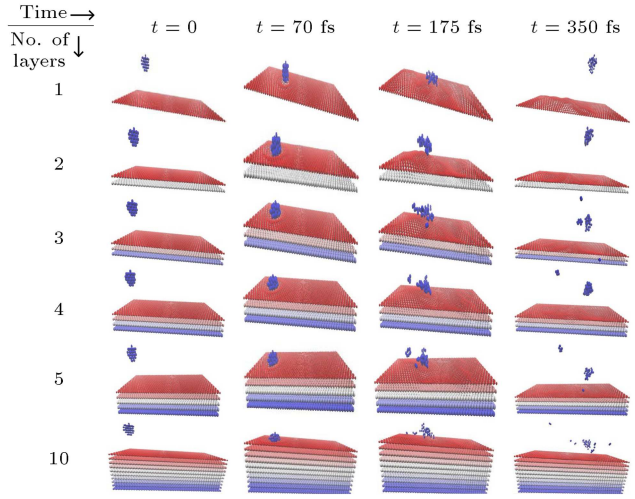

Figure 11. Deformation of metallic particles impacting on single- and various few-layer graphene sheets along the simulation time ($\theta = 30^\circ$).

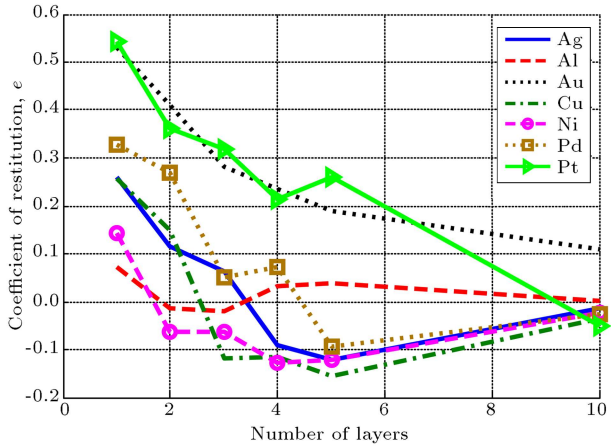

Figure 12. Effects of the number of layers on the normal coefficient of restitution for metallic nanoparticles.

were higher than those of other materials. As an interesting observation, some cases had negative normal coefficients of restitution. This issue has been reported in previous works on nanostructures [8].

Figure 13 shows the tangential coefficient of restitution. Because of unchanged direction of x-component particle's velocity, all values are negative. Tangential

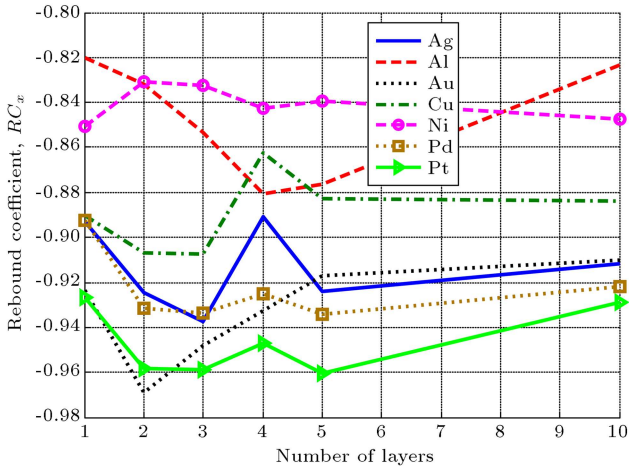

Figure 13. Tangential coefficient of restitution for graphene sheets under firing by various metallic nanoparticles.

coefficient of restitution did not change significantly by increasing the number of layers, though some fluctuations were observed locally.

From the presented figures, as a final classification, normal and tangential coefficients of restitution for the simulated materials can be listed as in Table 2. In this table, energy loss due to the impact has been calculated as $\Delta E = \frac{v_0^2 - v_i^2}{v_i^2}$ along 'x' and 'z' axes. Total energy loss was determined by summation of energy losses along those axes. For other impact angles, the same table and diagrams can be introduced.

Energy loss along 'z' axis is about 4 times greater than energy loss along 'x' axis. This is in agreement with the previous section, where at $\theta = 0^\circ$, horizontal impact velocity was zero and the vertical one, which contributed solely to the dynamics and normal coefficient of restitution, was in the range of $0.1 \sim 0.4$.

When impact velocity exceeds a critical value, the barrier will be ruptured and the projectile would pass through it. Such dynamics cannot be modeled via the classical mechanics; but, it is possible to do so by using NEMD (Non-Equilibrium Molecular Dynamics). Figure 14 shows the ruptured structure of a two-layer graphene sheet being impacted by a nanocluster. The images show the rupture structure after the nanocluster

Table 2. Classification of effects of number of layers on the normal and tangential coefficients of restitution ($\theta = 30^\circ$).

Metal	e	$\lvert RC_x \rvert$	ΔE_x	ΔE_z	ΔE
Ag	$6933e^{-0.31NL} - 6932e^{-0.31NL}$	0.91	-0.1650	-0.9819	-1.1468
Al	$-0.0027NL^3 + 0.043NL^2 - 0.18NL + 0.2$	0.75	-0.3825	-0.9986	-1.3811
Au	$0.68e^{-0.35NL} + 0.049e^{0.059NL}$	0.93	-0.1285	-0.8946	-1.0232
Cu	$-1935e^{-0.34NL} + 1936e^{-0.3413NL}$	0.89	-0.2097	-0.9765	-1.1862
Ni	$0.01NL^2 - 0.12NL + 0.21$	0.84	-0.2934	-0.9901	-1.2834
Pd	$1.3 \times 10^4 e^{-0.25NL} - 1.3 \times 10^4 e^{-0.256NL}$	0.92	-0.1478	-0.9674	-1.1152
Pt	$2.7 \times 10^4 e^{-13.44NL} + 0.65e^{-0.25NL}$	0.95	-0.1037	-0.8931	-0.9968

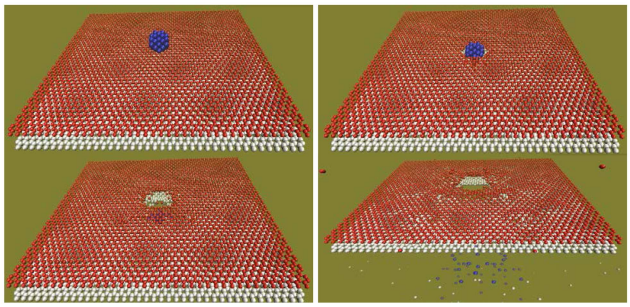

Figure 14. Ruptured structure of a two-layer graphene sheet before being impacted by a gold nanocluster (flexible), after passing the first layer, after passing the second layer, and after getting far away from the graphene sheet.

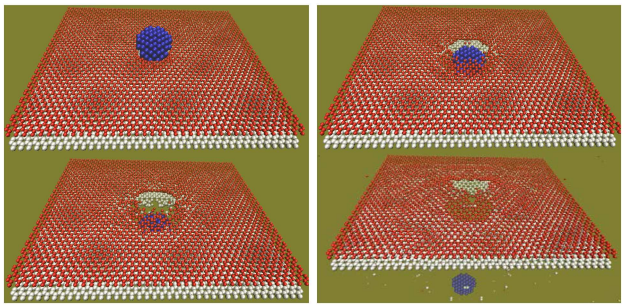

Figure 15. Ruptured structure of a two-layer graphene sheet before being impacted by a relatively rigid nanocluster, after passing the first layer, after passing the second layer, and after getting far away from the graphene sheet.

passes through the first layer and the second layer, and after it gets far away from the graphene sheet. Figure 15 repeats the figures for shooting a relatively rigid nanocluster (with scaled depth of the potential well (ε)). At the same time, more regular rupture could be observed with more rigid nanoclusters. More detailed studies could be suggested to classify the problem more and more.

Based on the conducted analysis, the problem of metallic nanoparticles impact on a graphene sheet can be modeled by classic mechanics and it would provide a simple and applicable model. Although for using this approach in complex systems with external effects, a different analysis is needed, this approach can still be considered as a reliable method to solve impact problems related to systems based on graphene in classic mechanics.

5. Conclusion

Impact theory was divided into four major aspects and classical mechanics was selected as the first aspect to predict the impact dynamics of graphene-based structures. Non-Equilibrium Molecular Dynamics (NEMD) approach was used and metallic nanoclusters were thrown onto various graphene sheets. The presented approach was validated and at the end, several useful results were presented that can be listed as follows:

1. Validation:
   a. Comparison of specific penetration energies. The specific energy dissipations, $E_p^* = E_p (\rho A_s h_{\text{ave}})^{-1}$, of single- to 20-layer graphene sheets were compared with those in an experimental work reported in [2]. Graphene sheets have considerably higher resistance against the projectile than metal micro plates;
   b. Comparison between deflections of the graphene. Mean deflections of graphene sheet at various times due to the shooting of argon clusters were compared with those in a previously simulated problem in [7]. It was observed that for higher velocities, the argon cluster exploded; therefore, comparison was not possible, exactly, same as what has been reported in [7].
2. Effects of impact velocity:
   a. By increasing horizontal impact velocity, the tangential coefficient of restitution decreases, whereas the normal coefficient of restitution increases. This is due to the momentum-related resistance of SLG against the faster impacted projectile;
   b. For macro bodies, the normal coefficient of restitution depends on the impact velocity and it approaches zero when the impact velocity increases. It was demonstrated that such behavior is not valid in the case of collision of nanoparticles with graphene sheets.
3. Effects of impact angle:
   a. Approximately, all the particles had the same trend with different mean values for normal coefficient of restitution;
   b However, normal coefficient of restitution for aluminum was almost constant, whereas other materials followed the fitted quadratic equation as: $e(\theta) = 0.418\theta^2 - 0.045\theta - 0.396$, where unit of θ is radian;
   c. In the comparison of tangential coefficients of restitution, except aluminum, which behaved completely different, other materials followed a fitted cubic relation as: $RC_x(\theta) = -0.9121\theta^3 + 2.371\theta^2 - 1.857\theta + 1.267$, where unit of θ is radian.
4. Effects of number of layers of graphene sheets:
   a. Increasing the number of layers decreases the normal coefficient of restitution;

b. Normal coefficient of restitution is higher for gold and platinum particles; but, for other metals, it is almost in a same specific range;

c. Negative normal coefficient of restitution has been observed for some cases, like what has been reported in some other works;

d. Tangential coefficient of restitution does not change seriously with increasing the number of layers, though some fluctuations are locally observed;

e. Based on the presented figures, normal and tangential coefficients of restitution for different materials are classified in a table;

f. Energy loss along 'z' axis is about 4 times greater than energy loss along 'x' axis. This is in agreement with the previous section, where at $\theta = 0^\circ$, horizontal impact velocity was zero and the vertical one has contributed to the dynamics. Coefficients of restitution were about $0.1 \sim 0.4$.

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Biography

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