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Resistance and rupture analysis of single- and few-layer graphene nanosheets impacted by various projectiles

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ABSTRACT

In this paper, a quasi-classical model for the collision of various nanoparticles with single- and few-layer graphene nanosheets was introduced as a multi-scale approach that couples non-equilibrium molecular dynamics with the Finite Element Method. As a resistance criterion, it was observed that the coefficient of restitution and the induced stresses depend on the impact velocity of projectile. These parameters were evaluated computationally, and it was revealed that certain resulting behaviors differ from behaviors at the macro scale. By obtaining an out-of-plane yield stress limit of 1.0 *TPa* for graphene, the stress analysis of single- and multi-layer graphene sheets revealed that the limit projectile velocity needed for the yielding of graphene sheets increases with the increase in the number of layers. For aluminum nanoparticles, this increase is almost linear, and for other metals, it slightly deviates from the linear trend. It was also observed that the graphene sheets have a different rupture form when impacted by gaseous molecules than by metal particles. Considering the very high momentum of gas molecules and their shock-like behavior during high-speed collisions with a graphene sheet, pores with a size of one carbon atom can be created in graphene sheets. Since a single-layer graphene sheet can withstand a projectile which is 3.64 times larger than a projectile impacting a 20-layer graphene sheet, spaced graphene sheets seem to be more effective in absorbing the impact energy of projectiles than conventional few-layer graphene sheets.

1. Introduction

Collision between two or several particles is one of the most fundamental problems in physics, and it is also important in chemistry, engineering, and some other fields. Advanced materials contribute significantly to impact related applications [1]; thus, impact analysis and especially the calculation of restitution coefficient is essential for measuring the operational efficiency of these materials. Graphene, formed as a single or few layers of carbon atoms in a honeycomb configuration, is as an amazing technology-based material with a great potential for withstanding the impact of projectiles. In ballistic tests, graphene sheets with a thicknesses range of 10–100 nm (equivalent to 30 to 300 graphene layers) have shown to have a high strain rate capacity [1]. The specific penetration energy for Few Layer Graphene Sheets (FLGSs) has been found to be ~10 times higher than that reported in the literature for macroscopic steel sheets at an impact velocity of 600 m/s [1]. In another

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research, the bombardment of a suspended monolayer graphene sheet by different energetic atoms has been studied via classical molecular dynamics based on the reactive force field (ReaxFF) [2]. As one of the most basic concepts of mechanics, Newton introduced a parameter called 'coefficient of restitution', to address the impact of macroscopic bodies. According to its standard definition, coefficient of restitution is the ratio of the normal component of rebound speed V_2, to impact speed V_1, when the impacted object is fixed ($e = V_2/V_1$). Recently, researchers have described the coefficient of restitution of objects in impact with graphene layers [3]. Based on the continuum model of particles, they have developed the theory of oblique impacts. Good agreement between the so-called macroscopic theory and simulations has been reported; which has validated the macroscopic concepts of elasticity, bulk viscosity and surface tension for nanoclusters of a few hundred atoms [3,4]. Some studies have investigated the collision of nanoclusters with graphene sheets [3–6]. Furthermore, the dynamic impact responses of Bucky balls (from C_{60} to C_{720}) have been investigated using molecular dynamics (MD) simulations [7].

In this paper, by using molecular dynamics simulations coupled with Finite Element Method to set up a multiscale approach, the collision of various molecules and metallic nanoparticles with graphene (single-layer) sheets has been studied. The effects of the number of layers, impact angle and impact velocity have been investigated, and some useful results have been obtained.

2. Modeling

In order to achieve a direct link between graphene sheets at the nanoscale and FLGS field at the microscale, a multiscale computational setup has been tested here. In this approach, the large and small computational systems are independent of each other, and they are only related through an iterative update of their boundary conditions. LAMMPS was used to solve the MD problem; and a written FEM code was employed to update the interfacial values with more flexible options.

Using inexpensive synthesis techniques, single-layer graphene sheets with few (less than ten) layers can be produced [8]. This may result in a lower resolution and sensitivity of the systems that are based on this type of graphene. For example, a nanoparticle placed on a graphene laminate affects the sheet with bonding forces that depend on the distance between nanoparticle and graphene laminate and on the type of material on both sides, which is usually modeled as a Lennard-Jones (LJ) potential. For a macro model including several particles between the graphene sheet layers as well as a projectile impacting the MLGS, the equations of motion and the relevant boundary conditions could be derived by writing the equations for potential and kinetic energies and using the generalized Hamilton principle for a laminated shell segment.

The strain energy of a sheet is expressed as [9].

$$U = \frac{1}{2}\int \sigma_f^T \varepsilon_f dV + \frac{\alpha}{2}\int \sigma_c^T \varepsilon_c dV \tag{1}$$

where flexural stresses and strains are expressed as

$$\sigma_f^T = \begin{bmatrix}\sigma_x & \sigma_y & \tau_{xy}\end{bmatrix} and\ \varepsilon_f^T = \begin{bmatrix}\varepsilon_x & \varepsilon_y & \gamma_{xy}\end{bmatrix} \tag{2}$$

and the transverse stresses and strains are

$$\sigma_c^T = \begin{bmatrix}\tau_{xz} & \tau_{yz}\end{bmatrix} and\ \varepsilon_c^T = \begin{bmatrix}\gamma_{xz} & \gamma_{yz}\end{bmatrix} \tag{3}$$

Parameter α is known as the correction factor, and considered as 5/6 [9]. By assuming the first-order shear theory, three degrees of freedom (rotation about the y-axis (θ_x), rotation about the x-axis (θ_y) and vertical deviation along the z-axis (w)) can be considered for each point. With these assumptions, and with regards to the first-order shear theory, the strains in different directions will be as follows:

$$u = z\theta_x \quad v = z\theta_y \quad w = w_0 \tag{4}$$

Then, the bending strains will be