Shock responses of graphene reinforced composites via molecular dynamics simulations

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Abstract. Shock responses of graphene reinforced composites are investigated using molecular dynamics simulations. The first case studied is the response of spaced multilayer graphene plates under normal impact of a spherical projectile, focusing on the effect of the number of graphene monolayers per plate on the penetration resistance of the armor. The simulation results indicate that the penetration resistance increases with decreasing number of graphene monolayers per plate. The second case studied is the penetration resistance of laminated copper/graphene composites. The simulation results demonstrate that under normal impact by a spherical projectile the penetration resistance of copper can be improved significantly by laminating the copper plates with graphene. The results of this research have revealed the possibility that graphene might be used in hyper velocity-relevant armor systems to enhance their penetration resistance.

1. Introduction

Graphene has drawn great attention since it was fabricated in the laboratory [1,2]. Lee et al. [3] measured a Young's modulus of 1.0 TPa and a ultimate tensile strength of 130 GPa for monolayer graphene using atomic force microscope (AFM). Frank et al. [4] measured the effective spring constants of stacks of suspended graphene sheets using AFM. They found the spring constants ranging from 1 to 5 N/m for suspended graphene sheets less than 10 nm thick. And they also extracted a Young’s modulus of 0.5 Tpa, which is significantly below the monolayer value of 1.0 Tpa. Marianetti and Yevick [5] have determined the failure mechanisms of pure graphene in a generic state of tension at zero temperature. The usual elastic instability causes failure for strains near uniaxial and a novel soft-mode phonon instability of the K1 mode causes failure for strains near equibiaxial.

Using spaced plates instead of a monolithic one to increase the penetration resistance of armor systems has being investigated for a long time. But there is no consensus in this area. Teng et al. [6,7] found that double-layer metal shield is able to improve the ballistic resistance by 8.0%–25.0% for a flat-nose projectile. But for a conical-nose projectile, it is almost as capable as the monolithic plate. Nia and Hoseinie [8] reported that single layer metallic targets have greater ballistic limit velocities than multi-layered targets under impact by hemispherical-nosed projectiles. So, whether the spaced plates or the monolithic plates are stronger is an open question. In this study, we will investigate shock responses of spaced multilayer graphene plates and compare the penetration resistance with each other.

The mechanical properties of laminated composites have been studied since several decades ago. Cook and Gordon [9] reported that strength and toughness of brittle solids could be largely increased if a plane of weakness or potential cleavage normal to the plane of the original crack is present. Yadav
and Ravichandram [10] found that penetration resistance of a pristine ceramic structure could be improved significantly by laminating ceramic tiles with thin polymer layers in between. Since graphene has extraordinary mechanical properties, we plan to investigate whether it can be used in composites to increase their penetration resistance.

2. Simulation methods

In this paper, molecular dynamics (MD) simulations are used to investigate the penetration resistance of spaced multilayer graphene plates and the laminated copper/graphene composites. The interaction between carbon atoms is calculated using the adaptive intermolecular reactive empirical bond-order (AIREBO) potential [11]. Copper atoms are described using the embedded atom method (EAM) [12]. The carbon-copper interaction is modeled using a Lennard-Jones form pairwise potential $V(r) = 4\varepsilon\left[(\sigma/r)^{12}-(\sigma/r)^{6}\right]$, and the parameters are $\varepsilon=0.0328$ eV, $\sigma=2.853$ Å [13].

3. Results and discussion

The models for spaced multilayer graphene plates are shown in figure 1. Each model contains totally 12 graphene monolayers divided into several spaced plates. The number of graphene monolayers per plate is denoted by $n$, and the distance between adjacent layers is 3.35 Å. Each graphene monolayer is circular in shape with a radius of 100 Å. A spherical diamond cluster with a radius of 15 Å is used as the projectile, which is fixed rigid with purely repulsive interaction with the target. Simulations are performed with an initial temperature of 300 K using an NVE ensemble.

![Figure 1. Simulation models for spaced multilayer graphene plates. The sphere on the left is the projectile, and the plates on the right are the graphene plates ($n$ denotes the number of graphene monolayers per plate).](image1)

![Figure 2. Ballistic limit velocity ($V_{bl}$) against the number of graphene monolayers per plate ($n$).](image2)

We calculated the ballistic limit velocity for each model using the same projectile. The ballistic limit velocity ($V_{bl}$) is the minimum velocity of the projectile required to perforate the target with a zero residual velocity [8]. The results are illustrated in figure 2, which demonstrate that $V_{bl}$ increases with decreasing $n$. And the relationship between $V_{bl}$ and $n$ can be described appropriately by a second order
exponential decay fit. $V_{bl}$ is 13.0 km/s in the case of n=12. But in the case of n=1 it increases to 20.0 km/s, 53.85% higher than the former case. In our simulations the system with one graphene monolayer per plate has the highest penetration resistance. Because in the system n=1 the distance between adjacent graphene layers is large enough to avoid interactions between them. Therefore, the target could have sufficient tensile deformation during the penetration process. Hence, we can speculate that the interactions between adjacent graphene layers reduce the strength and penetration resistance of the graphite target.

The penetration resistance of laminated copper/graphene composites has also been investigated. 5 types of model have been established. One is a monolithic copper plate with the size of $400 \times 400 \times 50$ Å$^3$ (figure 3(a)). The other 4 are copper/graphene composites with graphene layer on the impact (figure 4(a)) or back (figure 5(a)) surface, between 2 thin copper plates (figure 6(a)), and both on the impact and back surfaces (figure 7(a)). A spherical copper cluster with a radius of 20 Å is used as the projectile. We first obtain the critical velocity under which the monolithic copper plate has just totally been perforated (figure 3(b)). Then the projectile is given this critical velocity to impact other 4 composites.

In figure 3, (a) is the simulation model. (b) shows the configuration after the target has been totally penetrated. Different color represents different lattice structure. Blue is unknown, cyan is bcc, green is fcc and orange is hcp.(c) shows the dislocation distribution of the target. And the meanings for each parts in figures 4-7 are the same as in figure 3.

![Figure 3](image)

**Figure 3.** Result for pure copper plate. (a) Simulation model. (b) Configuration after the target has been totally penetrated. (c) Dislocation distribution of the target.

The results show that under normal impact with the critical velocity the 4 composites have very different responses from each other. For the composite with graphene on the impact surface the projectile fell to pieces and there formed a crater in the copper plate. In the case of graphene on the back surface there also formed a little crater in the copper plate. For the composite with graphene layer between 2 thin copper plates, the upper copper plate has already been perforated which is not the case for the lower plate. In the last case, in which graphene both lay on the impact and free surfaces the projectile fell to pieces and there is no perforation occured. In all these cases the graphene layer has no damage at all and the composite targets have not been totally penetrated. This phenomenon is reasonable because in this study the interaction between graphene monolayer and copper plate is described by a weak van der Waals force which couldn’t destroy the structure of graphene monolayer, hence the graphene layer could protect the copper plate since it has much higher tensile strength than
any other materials. We also found that the dislocation distributions are different from each other, maybe this is another possible reason for the enhancement mechanism.

**Figure 4.** Result for graphene lay on the impact surface of copper plate. (a) Simulation model. (b) Configuration at the time the target has maximum deformation. (c) Dislocation distribution of the target.

**Figure 5.** Result for graphene lay on the back surface of copper plate. (a) Simulation model. (b) Configuration at the time the target has maximum deformation. (c) Dislocation distribution of the target.
4. Summary
In summary, shock responses of graphene reinforced composites are investigated using molecular dynamics simulations. Simulation results for the spaced multilayer graphene plates indicate that under normal impact of a spherical projectile the penetration resistance increases with decreasing number of monolayers per plate, and the system with one graphene monolayer per plate has the highest penetration resistance. In the case of laminated copper/graphene composites, the results show that...
under normal impact by a spherical projectile the laminated copper/graphene composite has much higher penetration resistance than the monolithic copper plate.

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