Mechanical response under ballistic impact of penta-graphene

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INTRODUCTION

Recently, Shunhong Zhang et al[1] proposed a new class of carbon-based nanostructures, named 'penta-graphene' (Fig. 1a-1b). In this work it is reported preliminary impact molecular dynamics results for a monolayer of penta-graphene. It was investigated the mechanical response of these structures under 'ballistic' impact of diamond fragment (entirely atomistic).

METHODS

The simulations were carried out using the LAMMPS[2], which is a very suitable and flexible package for high quality molecular dynamics simulations. The force field employed was AIREBO (Adaptative Intermolecular Reactive Empirical Bond-Oder) force field [3,4]. This kind of potential has some advantages: it allows the bonds breaking and re-bonding, and it is very accurate to model carbon-carbon atoms interaction. The choice of incident particle as a diamond fragment was because this material has a well-known large mechanical resistance.

It was simulated impact dynamics with several different velocities for incident diamond particle. It was compared results of impact dynamics for graphene and penta-graphene.

RESULTS AND DISCUSSION

In the Fig. 2, we show the kinetic energy evolution for a 4000 m/s (40A/ps) incident particle initial speed under collision. As can be observed, penta-graphene monolayer absorbs less impact energy than graphene monolayer. Our results show that penta-graphene monolayer is a good absorber of mechanical impact, although less efficient than graphene. While penta-graphene absorbed around 45% of impact energy, graphene absorbed around 95%.

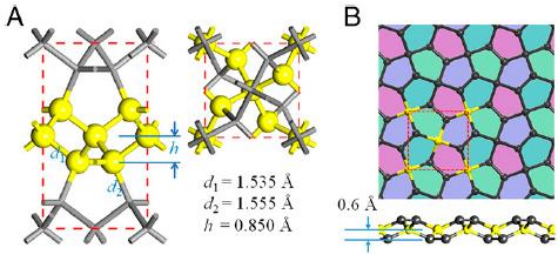

Figure 1. (a) Crystal structure, (b) top and side views of penta-graphene.

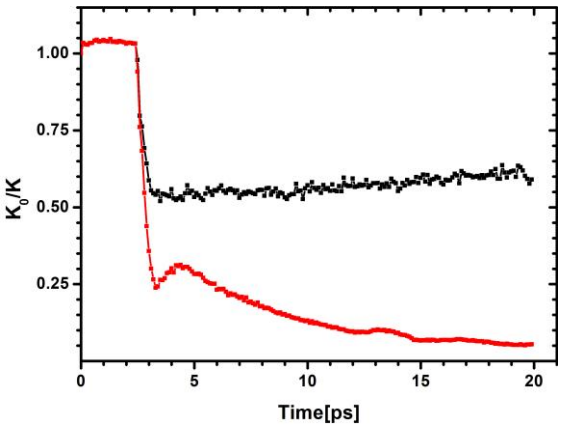

Figure 2. Temporal evolution of kinetic energy of incident particle of impact dynamics for a) black square, penta-graphene target, b) red circle, for graphene target.

CONCLUSIONS

The results presented here show that penta-graphene monolayer is a good absorber of impact, although is lesser efficient than graphene monolayer. The efficiency for penta-graphene energy absorption for this particular case of incident velocity(40A/ps) was around 45%.

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[1] Zhang, Shunhong; Zhou, Jian; Wang, Qian; et al., PNAS, 112, 2372 (2015).
[2] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J. Comp Phys, 117, 1-19 (1995).
[3] S. J. Stuart et al., J. Chem. Phys. 112, 6472 (2000).
[4] D. W. Brenner, Phys. Rev. B 42, 9458 (1990).