Plasma deposition and swift heavy ion irradiation effects of diamond-like-carbon coating multilayer graphene: A molecular dynamics simulation

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In spite of versatility of electronic properties of graphene [1], frangibility and low resistance to damage formation and external deformations reduce the practical value of this material for many applications [2]. To protect graphene from external influence, coating with thin layer of amorphous carbon is a viable solution against accidental scratches and other external random impacts [3]. Since graphene is also a promising material used in accelerators and in space in the future, it is of significant importance to study the property and structure changes of graphene and its protective amorphous diamond-like-carbon (DLC) coating after swift heavy ion irradiation.

In this study, we investigate the relationship between the deposition condition and quality of DLC on top of multilayer graphene by means of molecular dynamics simulations. Subsequently, we simulate swift heavy ion irradiation on the structure after deposition by utilizing two temperature model and further study the property and structure changes in both graphene and diamond-like-carbon coating.

Our simulation results reveal that lower temperature and incident energy will give higher sp^3 fraction in deposited DLC and it reaches highest of 16.68% when deposited by 70 eV carbon atoms at 100 K. Radial distribution function shows sp^3 hybridized carbon atoms tend to grow near sp^3 carbon atoms Ring analysis further indicates that diamond-like-carbon generated above sp^2 structures like graphene has more disordered ring structures. After swift heavy ion irradiation, temperature of DLC in the irradiation center can reach over 15000 K at the beginning of irradiation while there would be a low density and sp^3 fraction area left in the central region after 100 ps. According to track radius analysis after irradiation, DLC prepared under 70 eV carbon atoms bombardment will provide better protection to beneath graphene. High temperature annealing done to the irradiated multilayer graphene shows that although annealing can help to repair some vacancy defects by merging dangling atoms into the vacancy, it still leaves more chaotic interlayer connection and structure unexpectedly.

References

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