Tribological Properties and Mechanism of Graphene by Computational Study

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1. Introduction

Since graphene has been experimentally demonstrated to be the strongest material so far, it is motivated to play a wider role in nanomechanical applications. As a result, the tribological properties of graphene must be better understood. But there have been only a few tribological experiments by Atomic Force Microscope scratching, and due to the limitation of experiment, the fundamental tribological mechanisms are still not clear. In this paper, we carried out a molecular dynamics (MD) study and quantum chemical calculation of nanoscratching of graphene to investigate the dependence of friction force and friction coefficient on scratch depth, tip shape, scratch velocity and scratch direction. Furthermore we clarified the tribological mechanism of graphene by analyzing the relationship between atomic structure changes and the tribological properties.

2. Molecular dynamics model

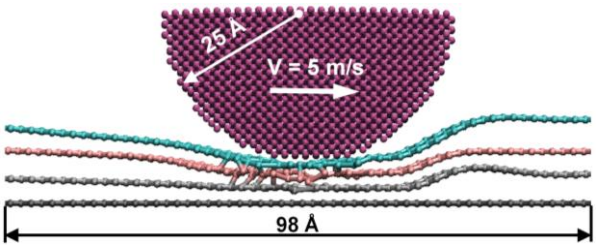

Figure 1. MD nanoscratching model of graphene

Figure 1 is the MD simulation model of nanoscratching of graphene. The tip first indents graphene, and after 100000 steps relaxation, the diamond tip begins to slide at a speed 5 m/s at different scratch depths. The tip is purposed to be rigid, the bottom layer and the boundary of grapheme are also fixed. The sizes of the system are shown in Figure 1. The interaction between the tip and graphene is described by Lennard-Jones potential. Meanwhile the graphene interlayer interactions are described by REBO potential. These potentials are widely used to calculate the interactions of C-C.

3. Results and discussion

Figure 2 shows the variation of friction force with the sliding distance under different scratch depths. With the increasing of the scratch depth, the friction force of the tip becomes larger. The force is almost zero when the depth is 4.48 Å. When the scratch depth is in the range of 4.48 Å and 5 Å, the curve of friction force is very smooth and showed sine periodicity. The period is about 2.45 Å, similar to the crystal parameter of graphene. This is because when the scratch depth is less than 5.0 Å, graphene only suffers to small depression deformation and the hexatomic rings are remained intact. Conversely, the regular lattice structure has influence on the friction force. As the scratch depth goes up to 5.3 Å, the friction force obviously ascends. During the scratching process, the bonds beneath the tip are broken and the instantaneous energy relaxation leads to the fluctuation of the friction force. The amplitude becomes much larger, and the periodic property is disturbed as well. After the scratching process, the structure recovers. However, if the scratch depth is 5.8 Å, graphene turns into amorphous and cannot recover. Then the average friction force reaches 80 nN, and the trend is without any periodicity which fluctuates even seriously.

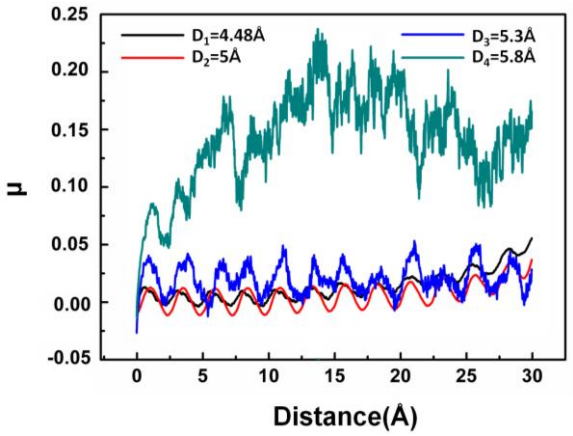

Figure 2. Under four scratch depths, the friction force of the tip varies with the sliding distance

4. Conclusions

We have carried out molecular dynamics simulations of nanoscratching on the multilayer graphene using diamond tip. In particular, the dependences of the friction force and friction coefficient on scratch depth, scratch velocity, scratch direction, and tip size have been studied. We find that the friction force of grapheme performs three distinct properties according to different scratch depths. The friction coefficient shows significant anisotropy. Also based on the atomic structure transformation, the mechanism of tribological properties is described.

5. Acknowledgement

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