New Potential of Graphene Layer for Controlling Nano-Wear

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1. Introduction

Since graphene successfully prepared experimentally, it has attracted a lot of attentions due to its excellent electrical and mechanical properties. In this paper, we proposed a new model to explore graphene layer new potential for controlling the surface nano-wear (defined by the number of sticking atoms) under C60 intrusion process by Molecular Dynamics(MD) approach. Furthermore, this study also explores a science problem on how C60(the smallest ball in nature) passes through a nano sliding contact space and how the graphene layer controlls the passing.

2. Molecular dynamics model

Figure 1 shows the MD model for the simulation, where three different models were proposed: Model-I, no substrate is layered by the graphene; Model-II, only the lower substrate is layered by the graphene; Model-III, both the substrates are layered by the graphene. The simulation sizes were given by $A_1 \times B_1 \times C_1$=108.6Å×43.4Å×16.29Å; $A_2 \times B_2$=102.09Å×43.31Å; $A_3 \times B_3$=47.97Å×21.30Å;$A_4 \times B_4 \times C_4$=48.87Å×21.72Å×10.86Å.

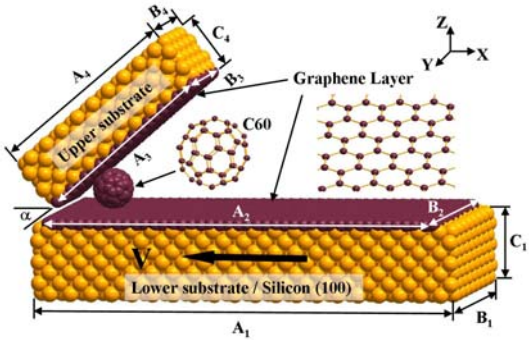

Fig. 1 MD simulation model for C60 ball intrusion a nano sliding contact space with graphene layers

The lower substrate was horizontal, while the upper substrate was inclined forming an initial entry angle α ranging from 20° to 90°. The atoms on the one outermost shell around the lower substrate as well as the atoms on the two rightmost shells of the upper substrate were fixed. The simulation was carried out using Tesoff potential of C and Si atoms at room temperature 300K. The lower substrate was moved at a constant velocity of 30Å/ps in the negative X-direction.

3. Results and discussions

Figure 2 shows the simulation results of Model-I, Model-II and Model-III when α is 40°, 80° and 90°, respectively. When α is 40°, the nano-wear(sticking atoms) of the upper substrate is most serious in Model-I; there are less sticking atoms in Model-II; the result is desirable that no atoms loss occurs in Model-III. These phenomenons are analogous when α is 80° and 90°, respectively.

From the results in Model-I and Model-II, it is observed that C60 can intrude the nano sliding contact space if α is 40° or 80°. However, when both of the substrates are layered by the graphene(see Model-III), C60 is always confined to the right side of the contact space whatever the initial entry angle would be. This means that graphene has the potential for defensing the nanoparticles intrusion a nano sliding contact space.

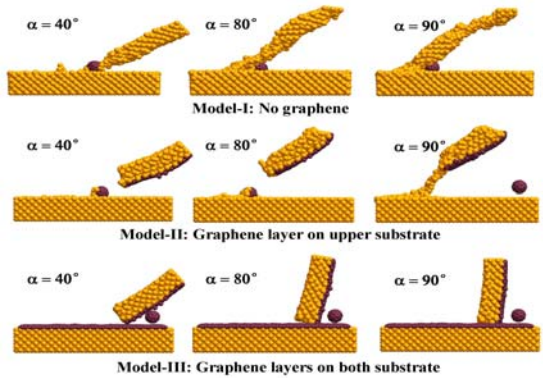

Fig. 2 The simulation results in case of initial entry angles 40°, 80° and 90° for three models

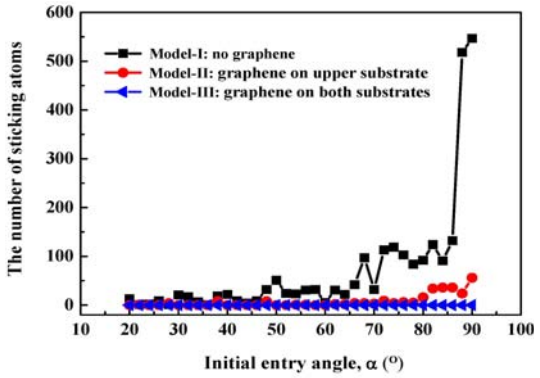

Fig. 3 The number of sticking atoms with variation of initial entry angles for three models

All the calculating results for the number of sticking atoms are summerized in Fig. 3. It is clear that the sticking atoms reduce obviously in Model-II, especially in Model-III the number of sticking atoms is zero. This means that graphene has a great potential for controlling the surface nano-wear.

On the other hand, according to the results in Figs.2-3, we found a critical initial entry angles 85° in Model-I and 82° in Model-II for C60 passing through the sliding contact space, respectively. When α is larger than the critical value, C60 can not intrude the sliding contact space. But for Model-III, no matter what initial entry angle, C60 can not intrude the space.

4. Conclusions

The new potential of graphene layer for controlling nano-wear was studied by Molecular Dynamics approach, in which two potentials of graphene layer were discovered. First, no wear of the substrate can be realized by using the graphene. Second, the graphene layer can be a promising matrial to defense the nanoparticles intrusion a nano sliding contact space. These findings may provide deep insights into the tribological behavior of graphene layered nano devices and lead to more widely applications of the graphene in nano mechanical system.

5. Acknowledgement

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