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Molecular dynamics simulation of AFM tip-based nanoscratching of multi-layer graphene

Pengfei Fan[1*], Ding Fan[2], Saurav Goel[3,4,5], Xichun Luo[1]

[1]*Centre for Precision Manufacturing, DMEM, University of Strathclyde, UK*
[2]*Shanghai Research Institute of Materials, Shanghai, 200437, China*
[3]*School of Engineering, London South Bank University, 103 Borough Road, London SE1 0AA, UK*
[4]*School of Aerospace, Transport and Manufacturing, Cranfield University, Bedfordshire, MK43 0AL, UK*
[5]*Department of Mechanical Engineering, Shiv Nadar University, Gautam Budh Nagar, 201314, India*

pengfei.fan@strath.ac.uk

Abstract
In this paper, molecular dynamic (MD) simulation was employed to simulate the AFM tip-based nanoscratching process on multi-layer graphene to investigate graphene deformation and coefficient of friction (COF). MD Simulation results showed cross-linking structures were created at the interface of two-layer graphene during nanoindentation and nanoscratching. The loading force had a characteristic of a periodic wave crest-trough transition. The COF of the diamond tip fluctuated at around 0.15 during nanoscratching process.

Keywords: Multi-layer graphene, AFM tip-based nanoscratching, MD simulation, Coefficient of friction

1. Introduction

Graphene is considered to be the most promising two-dimensional (2D) nanomaterial with unique physical chemical characteristics and wide application [1]. However, the zero bonding gap limits its application in electronic fields. Atomic force microscope (AFM) tip-based nanoscratching method is capable of nanomachining graphene and opening a proper bonding gap with nanoscale resolution [2]. However, it is extremely difficult to investigate graphene deformation and coefficient of frition (COF) of atomic level through experimental observation due to atomic layer to layer structure in the graphene. Molecular dynamic (MD) simulation has been proven as an effective technique to reveal the material deformation and COF in the atomic scale. Therefore, this paper employed the MD simulation to investigate the nanoindentation and nanoscratching process on multi-layer graphene using a diamond tip.

2. Modelling setup and Computational details

This paper utilized Atomsk [3] software to establish MD simulation model of AFM tip-based nanoscratching on multi-layer graphene, as shown in figure 1. The graphene workpiece (16704 atoms) consists of four layers graphene marked by the olivedrab colour atoms (1st layer), magenta colour atoms (2nd layer), green colour atoms (3rd layer), red colour atoms (4th layer). The layer spacing was set 0.34 Å. The 1st and 2nd layer graphene were set the Newton layer. The 3rd and 4th layer graphene were set the thermostat layer and boundary layer, respectively.

The yellow colour atoms represents the diamond tip (445 atoms). The diamond tip was placed at the 2 Å above the multi-layer graphene workpiece surface. The diamond tip performed nanoindentation first to a depth of 6 Å with 1 m/s velociety along the negative Y direction, which can lead to nanoscratch the two-layer graphene. The nanoscratching was implementing 5 nm scratching distance with 1 m/s velociety along the negative X direction. The two processes were carried out in large-scale atomic/molecular massively parallel simulator (LAMMPS) [4]. Additionally, this paper selected the the second generation of reactive empirical bond order (REBO) potential [5] to describe the interaction of multi-layer graphene workpiece. The Lennard-Jones (LJ) potential [6] was adopted to calculate the interaction between the diamond tip and multi-layer graphene workpiece. The simulation results were visualised and analyzed using Open Visualization Tool (OVITO) software [7].

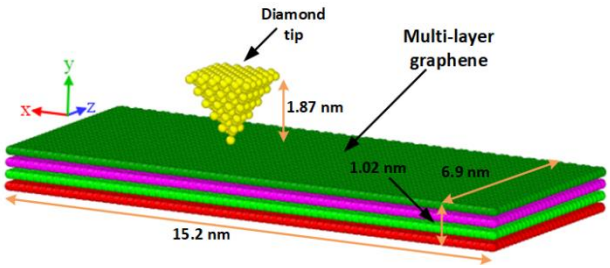

Figure 1. Three dimensional (3D) MD simulation model of AFM tip-based nanoscratching on multi-layer graphene

3. Results and discussion

3.1. Nanoindentation process

The morphology of nanoindentation caused by the diamond tip is shown in figure 2. It can be seen that a cross-linking structure was created between the 1st layer and 2nd layer graphene. Additionally, the C-C bonds only deformed to a certain extent instead of breaking during nanoindentation process. The load-displacement curve is illustrated in figure 3. It is clear to see that the wave crest-trough transition implied the sites for 1st layer and 2nd layer graphene, respectively.

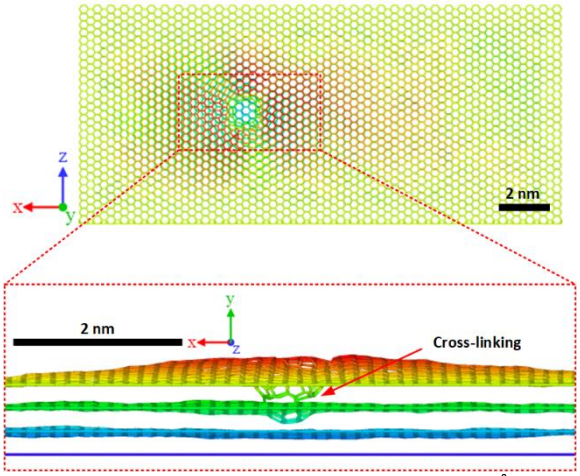

Figure 2. The morphology at nanoindentation depth of 6 Å

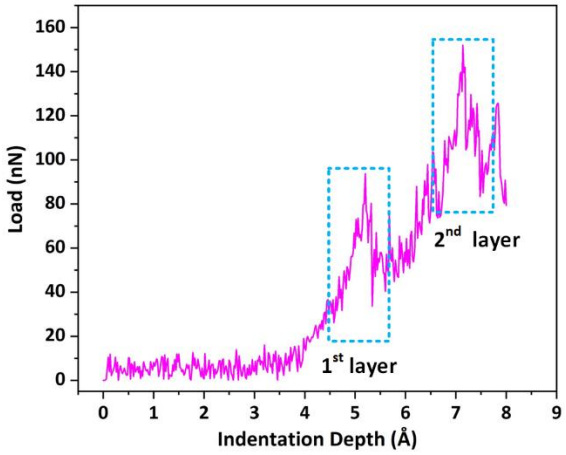

Figure 3. Load-displacement curve

3.2. Nanoscratching process

After conducting the nanoindentation, the diamond tip performed the nanoscratching with 5 nm distance. To this end, figure 4 shows the two layers graphene was scratched to create a obvious band gap by the diamond tip. Several C atoms in the 1st layer graphene combined with the C atoms in the 2nd layer graphene to form some amorphous carbon chain structures. Additionally, it is evident to see that the created cross-linking structures started to adhere to the surface of the diamond tip. The evolution of kinetic COF of the diamond tip with scratch distance is shown in figure 5. It was found that the COF experienced a fluctuation at around 0.15.

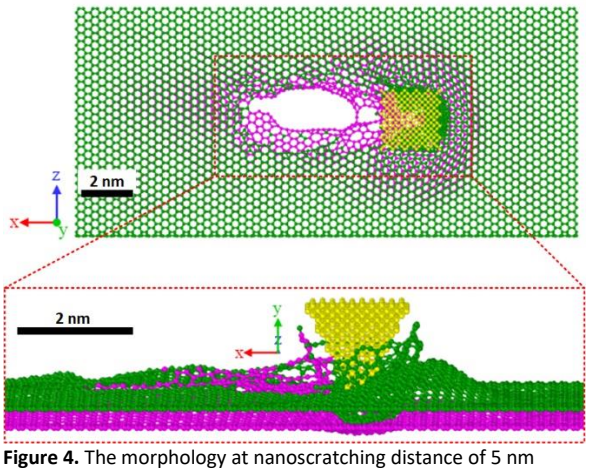

Figure 4. The morphology at nanoscratching distance of 5 nm

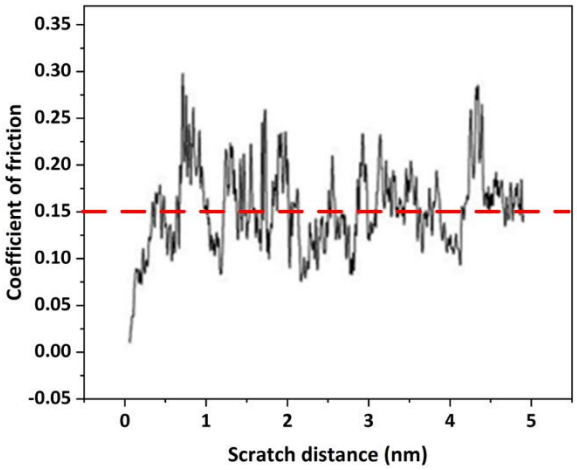

Figure 5. Variation of COF of the diamond tip with scratch distance

4. Conclusions

The MD simulation was employed to investigate the nanoindentation and nanoscratching process of multi-layer graphene using a diamond tip. The following conclusions can be drawn:

1. Cross-linking structures in two-layer graphene were created during nanoindentation and nanoscratching process, which could govern the COF. The loading force showed a periodic wave crest-trough transition, which indicates the sites of 1st layer and 2nd layer graphene.
2. The created cross-linking structures adhered to the surface of the diamond tip during nanoscratching process. The COF of diamond tip fluctuated at around 0.15 when nanoscratching two-layers graphene.

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