Understanding friction and wear at the nanoscale

Z. D. Sha*, P. S. Branicio, Q. X. Pei, J. Y. Zhang, V. Sorkin, and Y. W. Zhang

Institute of High Performance Computing, 1 Fusionopolis Way, 16-16 Connexis 138632, Singapore

Abstract

Friction and wear behaviors at the nanoscale have been investigated by molecular dynamics simulations. 1) For the wear law, the trend of lost-atom as a function of sliding distance indicates that the conventional macroscopic wear model (Archard's wear model) still works. 2) For the friction law, we investigated the contact mode with constant loading force. The relationship between contact-atom and the lateral force indicates that the number of chemical bonds between the tip and substrate is the dominant factor for the friction. Our work provides the fundamental understanding of friction and wear behaviors at the nanoscale.

1. Introduction

Understanding friction and wear at the nanoscale is important for many applications that involve nanoscale components sliding on a surface, such as nanolithography, nanometrology and nanomanufacturing [1]. It is normally believed that classic macroscopic friction and wear laws do not generally apply to nanoscale contacts. Although continuum mechanics models have been predicted to break down at the nanoscale, they continue to be applied for lack of a better theory [2]. An understanding of how friction force and wear depends on applied load and contact area at nanoscale is essential for the design of miniaturized devices with optimal mechanical performance. Here we use large-scale molecular dynamics simulations with realistic force fields to establish friction law and wear law in dry nanoscale contacts.

II. Computational details

In our molecular dynamics studies, we use bulk diamond-like carbon (DLC) as the substrate and the spherical DLC as tips (See Fig. 1). The DLC tips are prepared by cutting the desired shapes out of a bulk DLC sample. The potential we use the combination of Tersoff potential and *vdw* potential, instead of the second generation reactive empirical bond-order potential (REBO), because the Tersoff potential with enhanced cutoff has been proved to be the more accurate and efficient potential for amorphous carbon DLC. Simulations of normal loading are performed at 300 K by alternating loading, holding, and sliding phases. The sliding velocity is 20 m/s, which is comparable to the operating conditions in micromechanical systems (MEMS), but which is much larger than the typical velocity in scanning force microscopy (SFM) experiments.

II. Results and Discussion

1) For the wear law, the trend of lost-atom as a function of sliding distance indicates that the conventional macroscopic wear model (Archard's wear model) still works (See Fig. 2).

*E-mail address: shaz@ ihpc.a-star.edu.sg

2) For the friction law, we investigated the contact mode with constant loading force. The relationship between contact-atom and the lateral force indicates that the number of chemical bonds between the tip and substrate is the dominant factor for the friction (See Fig. 2).

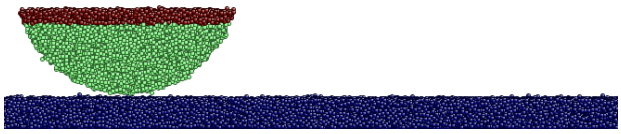

Figure 1

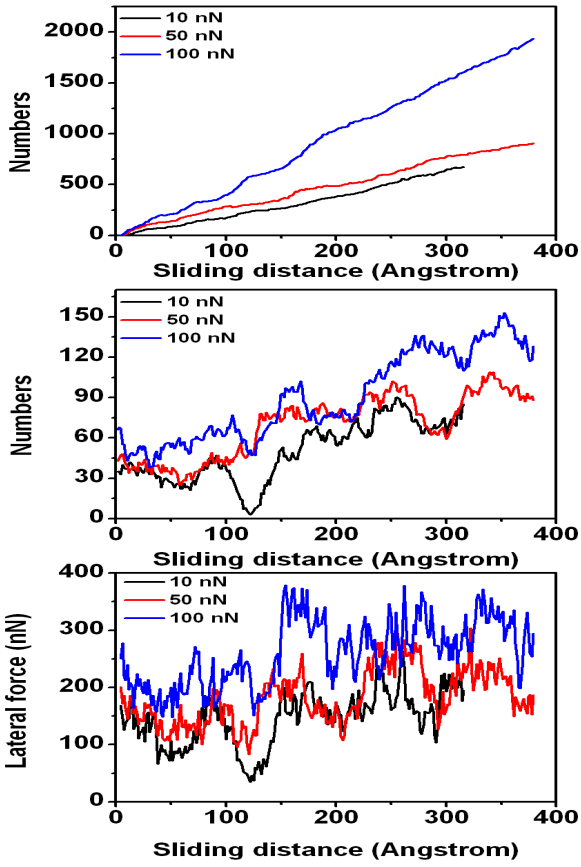

Figure 2

Reference

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