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# MOLECULAR DYNAMIC SIMULATIONS: THERMAL FLUCTUATIONS AND KINETIC FRICTION

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Recent development in nanotribology suggests that solid friction in nanoscale and atomic levels can be more complicated than Coulomb macroscopic laws. In particular, Ben-David and Fineberg showed how local normal load could affect the friction coefficient [1]. Therefore, the friction coefficient can be dependent on the contact area and the normal load. Indeed, the deviation from the Amontons' law has been reported in this research. In another study, for the case of thin films, friction is more like dissipation in liquids in the absence of a net normal load [2]. Consequently, more investigations on friction coefficient at the nano and atomic scales are of great importance.

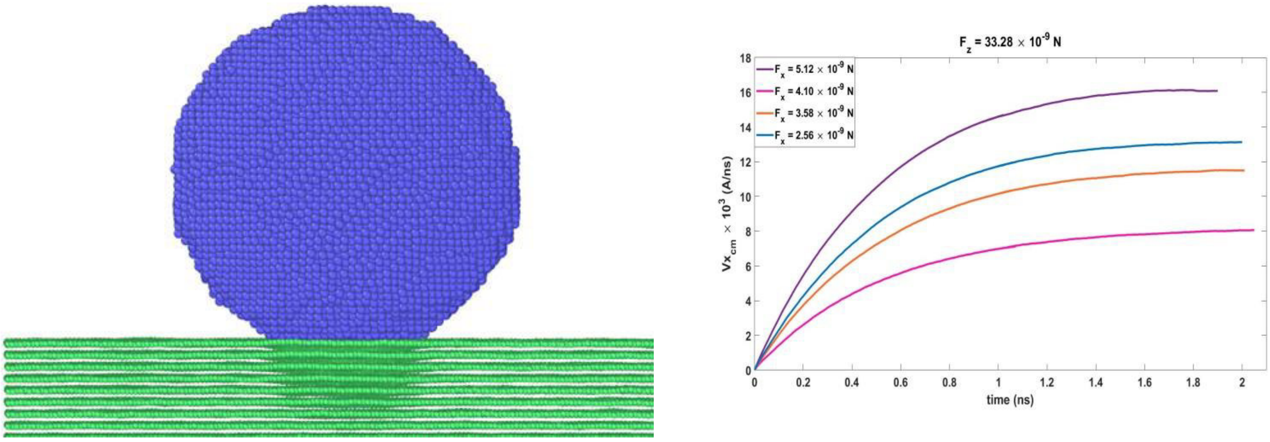
In this paper, molecular dynamic simulations are utilized to study friction at the nanoscale. The system has two parts as shown in Fig. 1a. Some graphene layers are utilized as a surface, and a spherical metal particle moves on the surface. In our case study, the spherical metal particle consists of roughly 32000 aluminum atoms in an FCC lattice. Besides, two forces are exerted on the particle; a normal load in the *z*-direction $F_z$, and a horizontal force, $F_x$, in the *x*-direction. The horizontal force provides movement for the particle on the surface. Moreover, a Langevin thermostat adds surface fluctuations in a nearly constant temperature.

In the theory, we consider a Langevin dissipation, $F_{fr} = \gamma v + \zeta(t)$, where $\zeta(t)$ is a random force with zero mean, $< \zeta(t) >$=0, according to the fluctuation-dissipation theorem. Fig .1b shows that the particle starts to accelerate and finally reaches a steady-state with a nearly constant velocity $<v(t)> \cong v$. At this point, the friction force $< F_{fr} >$ is equal to the horizontal force. That is $F_x = < F_{fr} >$. For this, one can investigate the linear proportionality of friction force on the velocity of the particle after reaching a steady state $v$. Namely,

$$F_x = \gamma\, v, \tag{1}$$

where $\gamma$ stands for the friction coefficient. Thereupon, simulated points will be velocities for different horizontal forces in a constant normal load.

As the first result, the friction coefficient will be evaluated by a linear fitting method for the simulated points. Fig. 2 illustrates the linear fitting for four realizations of Fig. 1b.




a b

Fig. 1. System (a) and an example for steady state (b)

As the second result, we have done simulations for different temperatures to investigate the thermal dependency of the friction coefficient. Fig. 3 shows that the friction coefficient decreases with increasing temperature.

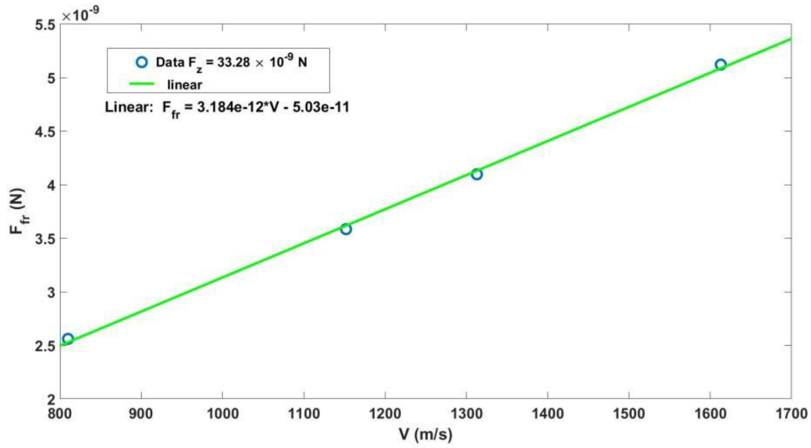



Fig. 2. Linear fitting for four realizations of steady states in a constant normal load $F_z = 33.28 \times 10^{-9}$ (N). The friction coefficient is $\gamma = 3.184 \times 10^{-12}$ (kg/s)

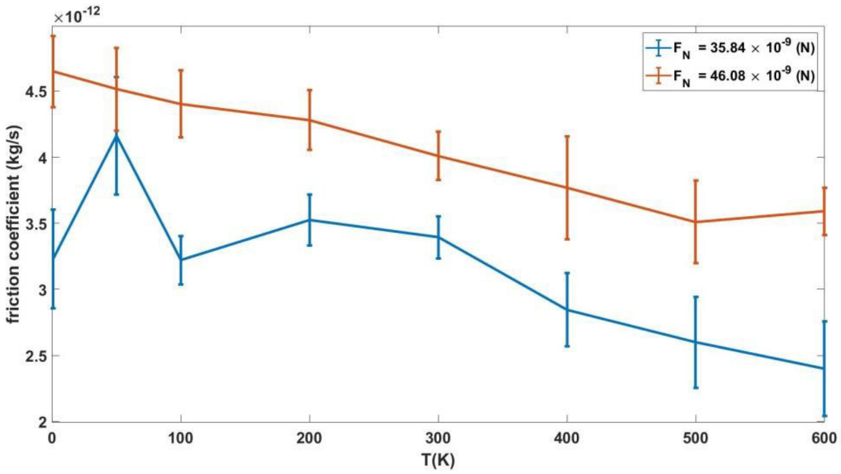



Fig. 3. Friction coefficient versus temperature. A reduction of friction coefficient observed with increasing temperature in a constant normal load

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1. Ben-David O., Cohen G., Fineberg J. The dynamics of the onset of frictional slip // Science. 2010. Vol. 330(6001). P. 211–214.
2. Krim J. Friction and energy dissipation mechanisms in adsorbed molecules and molecularly thin films // Advances in Physics. 2012. Vol. 61(3). P. 155–323.
3. Adinets A., Bryzgalov P., Voevodin V., Zhumatii S., Nikitenko D., Stefanov K. Job digest: An approach to dynamic analysis of job characteristics on supercomputers // Numer. Methods Program. Adv. Comput. 2012. Vol. 13. P. 160–166.
4. Zacharov I., Arslanov R., Gunin M., Stefonishin D., Pavlov S., Panarin O., Maliutin A., Rykovanov S., Fedorov M. "Zhores"— Petaflops supercomputer for data-driven modeling, machine learning and artificial intelligence installed in Skolkovo Institute of Science and Technology // Open Eng. 2019. Vol. 9. P. 512–520.