Сумський державний університет

Sumy State University

MOLECULAR DYNAMICS OF SHEAR OF ULTRATHIN FILM OF CARBON DISULFIDE BETWEEN DIAMOND SURFACES

Alexei Khomenko, Denis Boyko, Natalija Goncharenko, o.khomenko@mss.sumdu.edu.ua

Abstract

Using the method of classical molecular dynamics the tribological properties are studied of one molecular layer of liquid carbon disulfide, pressed by two atomically smooth diamond surfaces. We treat the models of elastic spheres for carbon disulfide molecules and absolutely rigid diamond plates. The found time series of atomic level friction force at the contact is heterogeneous. An increase of the external normal pressure leads to the transition of the film to a solidlike state. This is manifested in a decrease of the diffusion constant, in the behavior of velocity autocorrelation function of liquid molecules and average friction force.

Initial configuration

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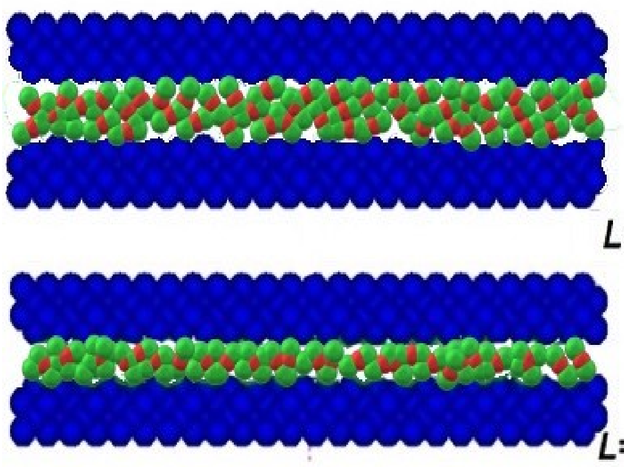
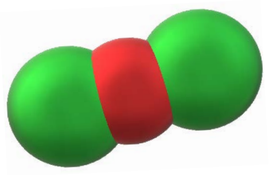


Molecule of carbon disulfide



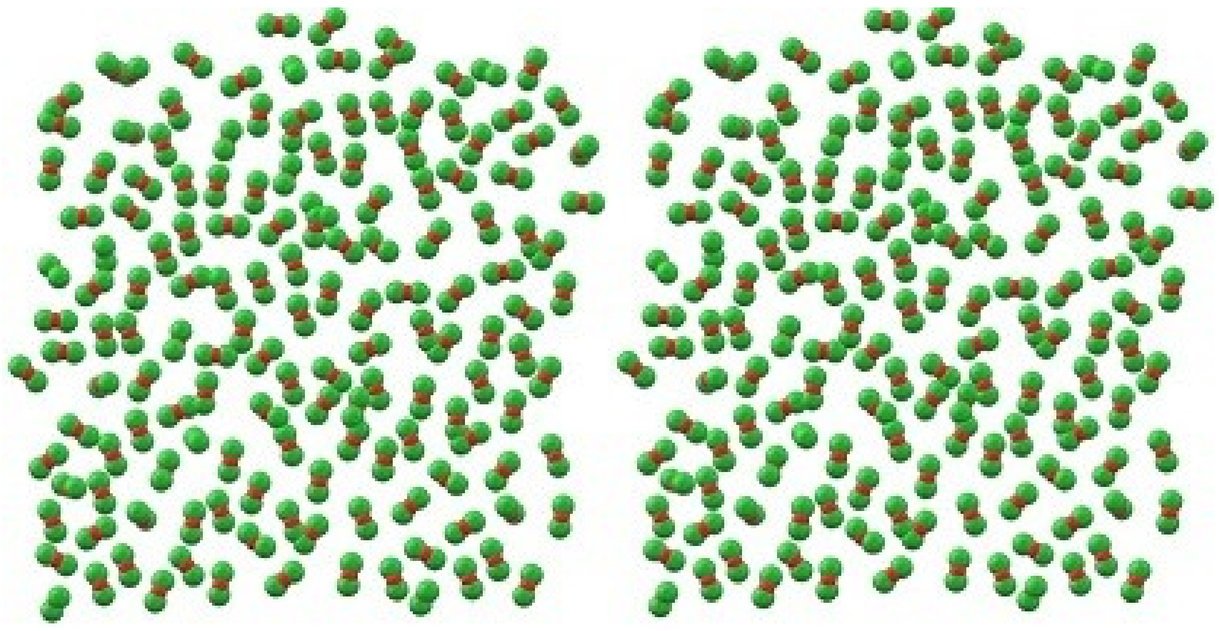
Interaction potential:

$$u_{ij} = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right], r_{ij} < r_c \\ 0, r_{ij} \geq r_c \end{cases}$$

Measures units: $F_0 = 3.42$ pN, $\varepsilon = 0.155$ kcal/mole, $t_0 = 5.253$ pN

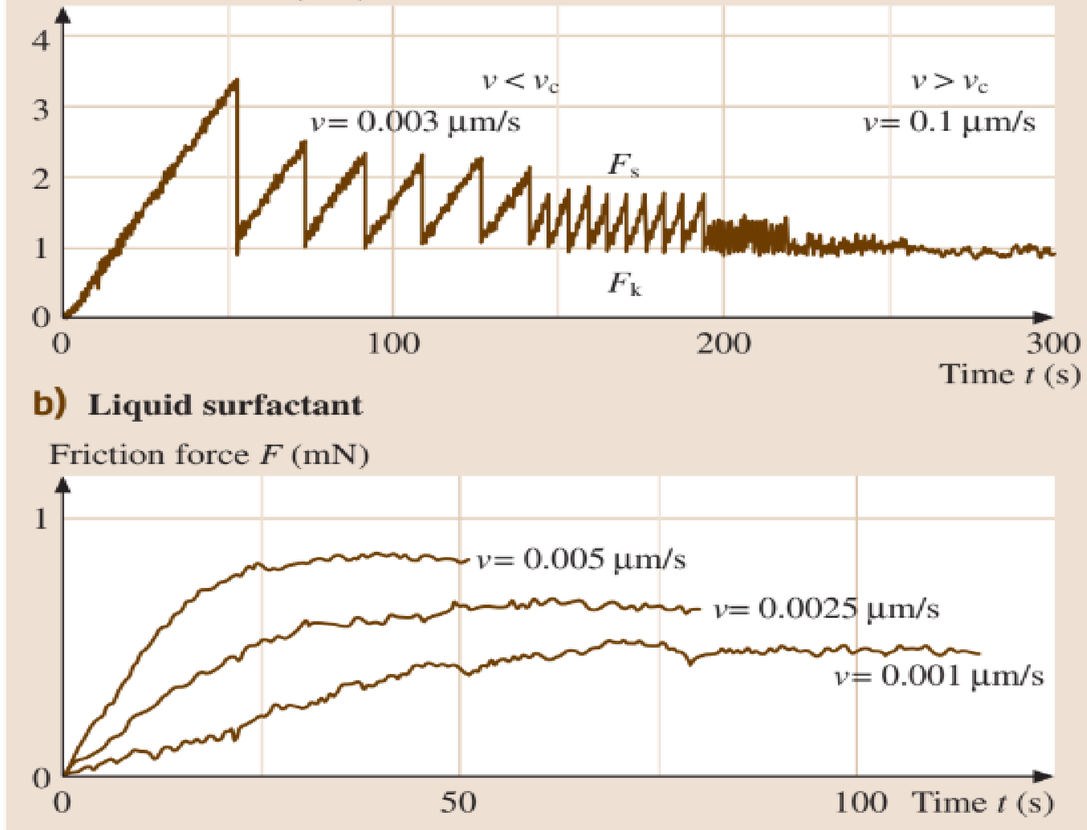
Time step: $\Delta t = 2.627$ fs

Typical molecules configurations L=0 and L=20



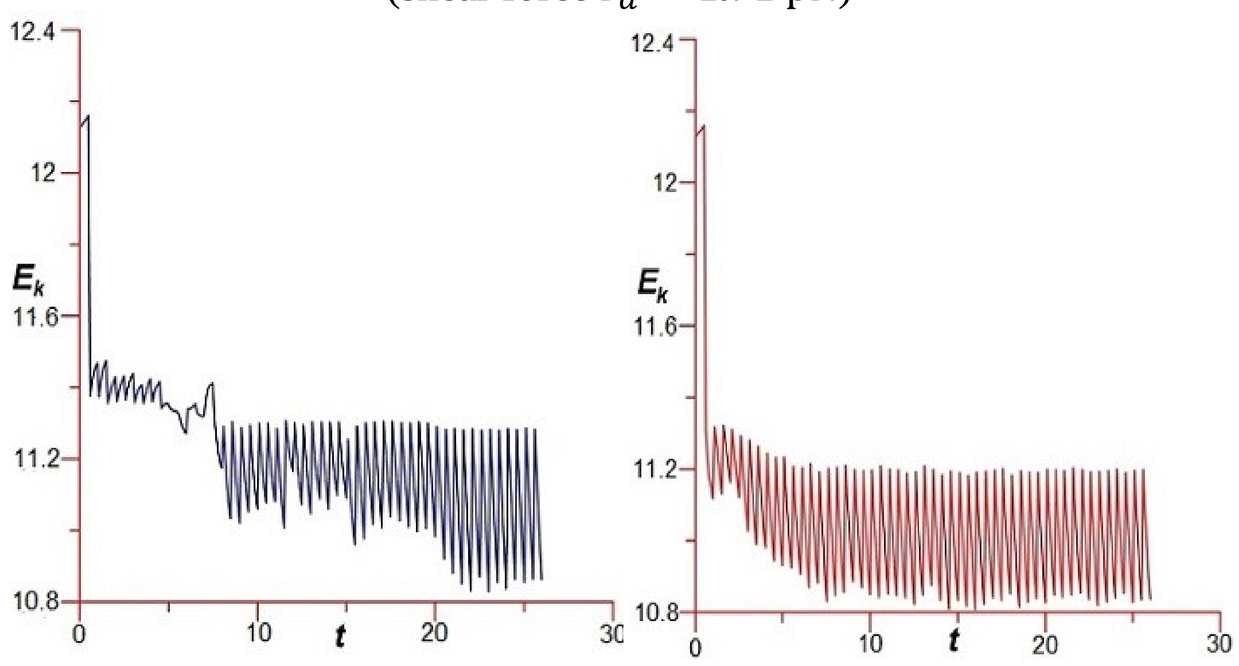
Experiment

B. Bhushan, Nanotribology and nanomechanics (Berlin: Springer-Verlag: 2005)

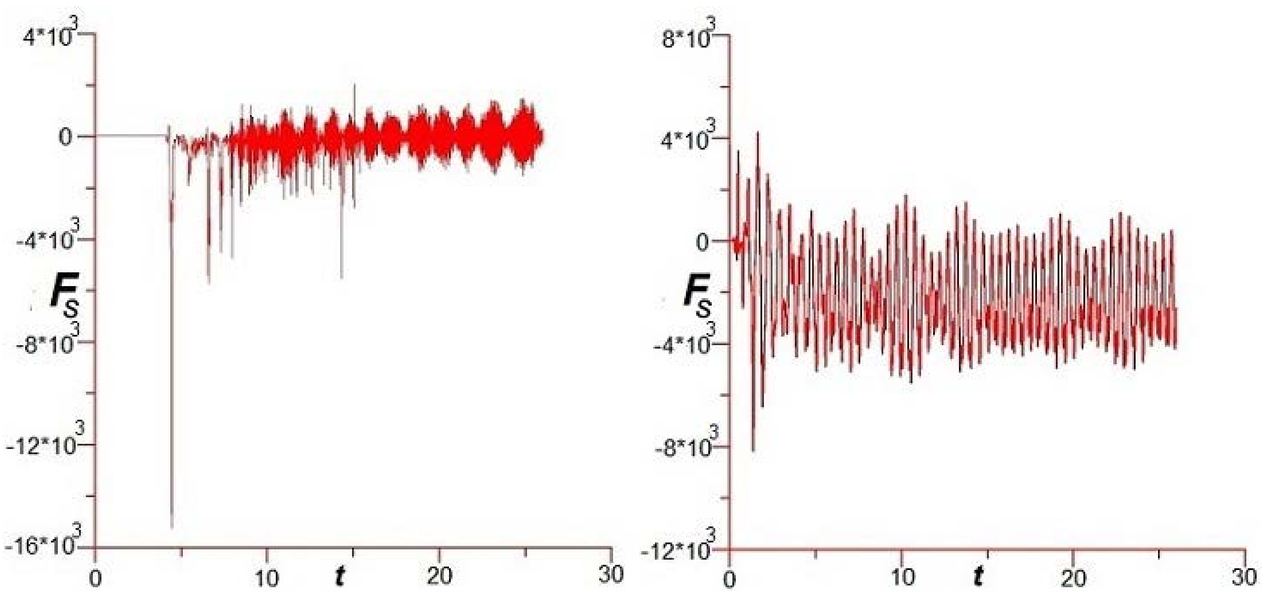


Measurements and results

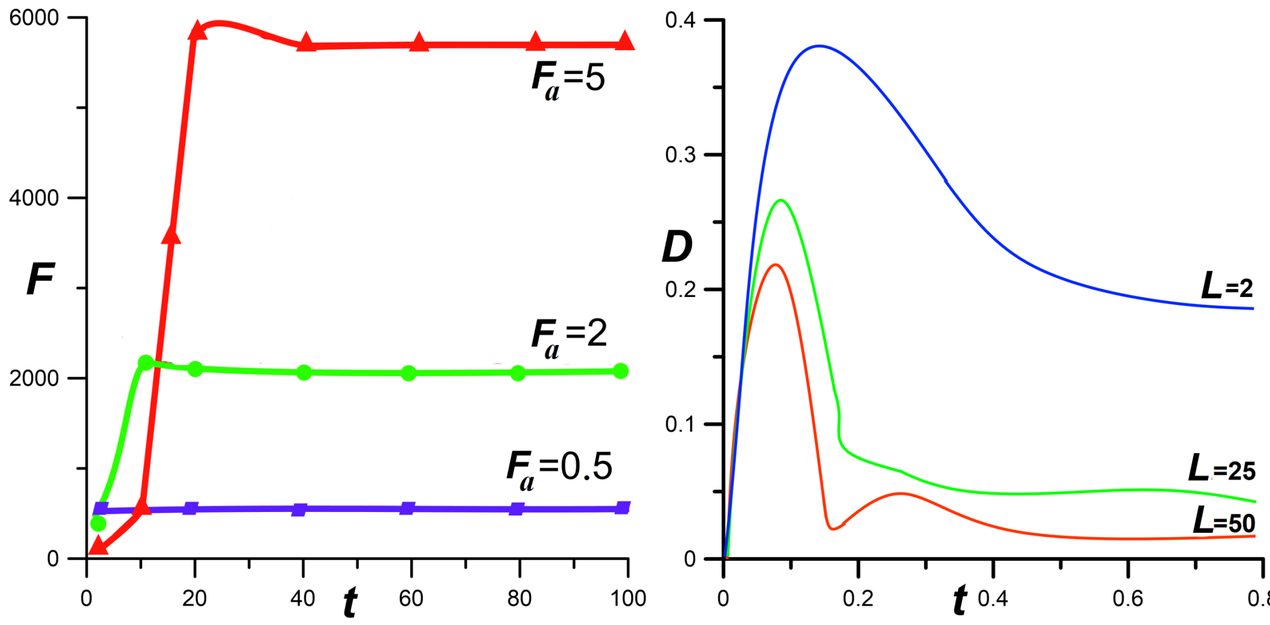
Time dependence of the kinetic energy at load L=0 and L=20 (shear force $F_a = 1.71$ pN)



Time dependence of the substrate force L=0 and L=20



Time-averaged value of the friction force and diffusion coefficient



Conclusions

It can be concluded from the study that the linear increase in the friction force with the load is not determined by the relief of the surfaces. This is explained by the rapid achievement of the saturation of the friction force with an increase in the load for all the models considered. Fluctuations of kinetic energy significantly increase the amplitude during the loading on the surface, this indicates an increase in the temperature of the liquid molecules. The main result of simulations is the transition of the ultrathin carbon disulfide film to a solidlike state. It manifests itself in the diffusion constant decreasing and in the ordering of molecules. One layer of molecules between flat rigid diamond plates behaves like simple Lennard–Jones boundary liquid lubricant and there is no expressed horizontal ordering in it. The presence of a driving force causes a more rapid formation of the ordered structures and the shear ordering takes place. The dependencies of time averaged values of friction force and shear stress are similar to the ones experimentally obtained for spherical molecules. They can be explained using the “cobblestone” model in the approximation of the adhesion forces domination.