SCIENTIFIC REPORT FOR SHORT VISIT GRANT

CONTACT MECHANICS AND ADHESION BETWEEN SELF AFFINE FRACTAL SURFACES

Vladimir N. SAMOILOV

Purpose of the visit

We plan to study contact mechanics and adhesion between self affine fractal surfaces using Molecular Dynamics.

The calculations will be performed with and without liquids between the solid elastic walls. The calculations will be for realistic solids with long-range elasticity. We will vary the fractal dimension and the root-mean-square roughness amplitude of the surfaces, and study how the contact mechanics and adhesion depend on these properties. The results will be compared to simple analytical models.

The results should be of great importance for MEMS applications and also for bio-adhesion where insects are known to inject thin liquid layers at the interface between the attachment organs and the rough substrate in order to increase the adhesion.

During the visit we planned to start this work. The whole simulations using Molecular Dynamics for systems including from 200000 to 300000 atoms are very time consuming. Thus we planned to prepare the systems and to start calculations in Juelich during this short visit and then to continue the work from Moscow.

Description of the work carried out during the visit

We used the modified version of the model that we have widely used in our Molecular Dynamics computer simulations of sliding friction, boundary lubrication, adhesion, squeezing of thin molecular films of lubricants and applications to wear (see Refs. [1-8]).

We concentrated on preparation of the systems without liquids between the solid walls. We prepared several systems with the flat elastically more soft block and the flat or corrugated rigid substrates. The idea was to come (in perspective) to the case with the rubber like block in adhesive contact with a hard rough substrate (see Fig. 1). Thus we were to come from the roughness of the

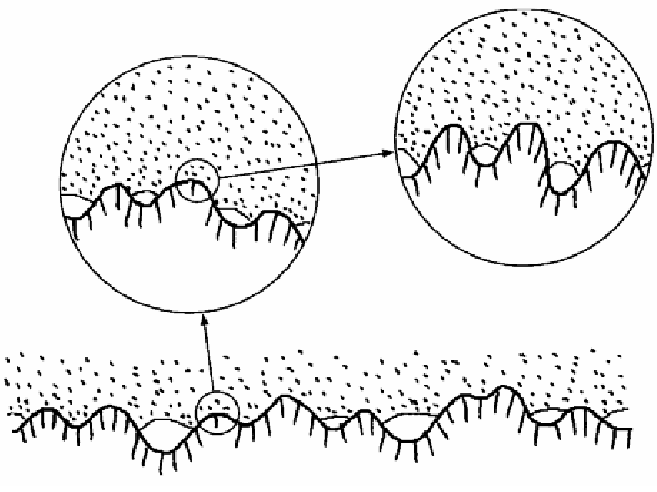

FIG. 1. A rubber block (dotted area) in adhesive contact with a hard rough substrate (dashed area). The substrate has roughness on many different length scales and the rubber makes partial contact with the substrate on all length scales. When a contact area is studied at low magnification it appears as if complete contact occurs, but when the magnification is increased it is observed that, in reality, only partial contact occurs. From [9].

substrate on one length scale (see, for instance, Refs. [7,8]) to the roughness of the substrate on many different length scales.

For this purpose we generated a number of self affine fractal rough substrate surfaces. One of these surfaces is presented in Fig. 2.

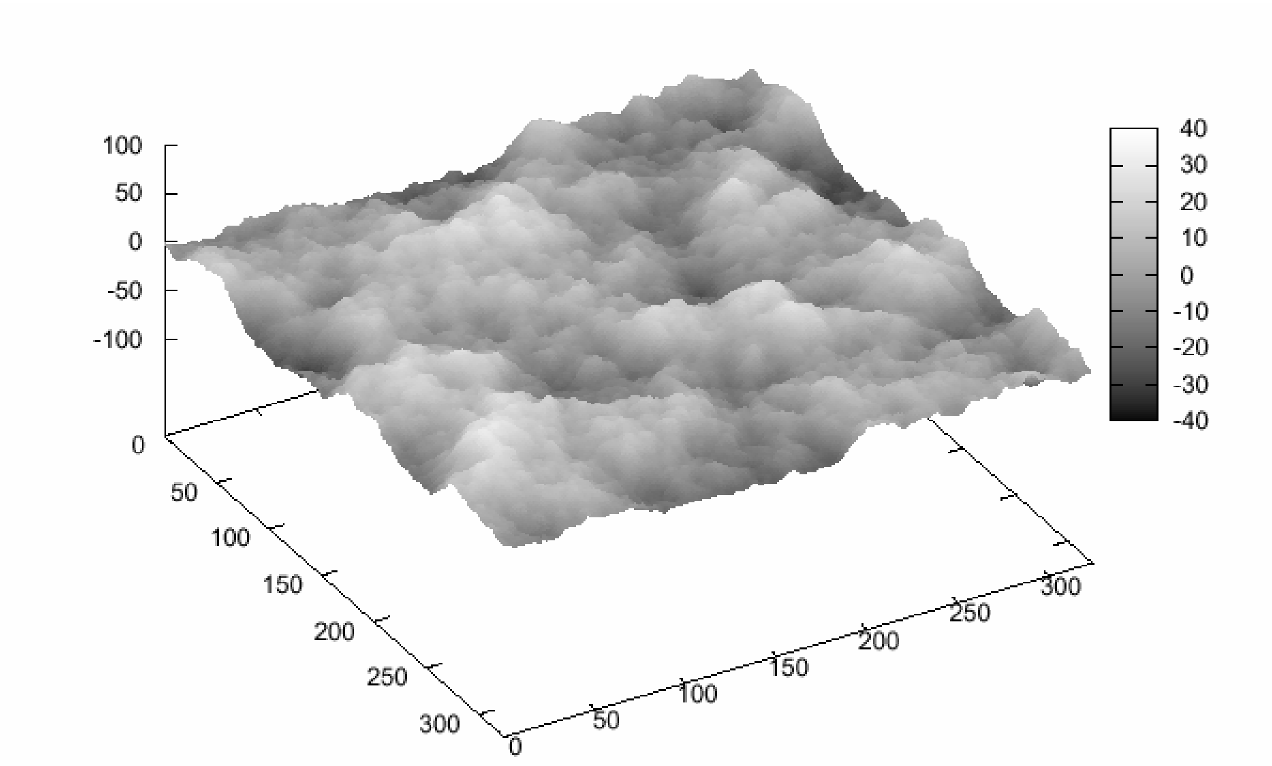

FIG. 2. One of the self affine fractal rough substrate surfaces generated during the visit. The surface has the root-mean-square roughness 10 Angstrom and Hurst exponent H = 0.8. Lengths in the picture are measured in interatomic distances. The number of atoms in the substrate surface 324*324.

We used the block with long-range elasticity with elastic modulus $E = 10^9$ Pa. This is intermediate between metals (used in Refs. [1-8]) and elastically soft rubber.

All the systems (with flat and self affine fractal substrates) were carefully prepared and their temperature was controlled in time to reach 300 K.

The surfaces were put into contact and then simulations were performed of further approach of the block towards the substrate. Thus we got the average pressure at the contact as a function of distance (time) and the snapshots of evolution of the contact region in time. Some of these simulations are still in progress now. We vary the fractal dimension and the root-mean-square roughness of the substrate and study how the contact mechanics depends on these properties.

Then we started the retraction and calculate the variation of the average pressure developed as the block moves away from the substrate. This will give the results on how the adhesion depends on the fractal dimension and the root-mean-square roughness of the substrate.

And finally we started the lateral motion of the block at certain applied external pressure values. We study the mechanism of friction and how the friction force depends on the fractal dimension and the root-mean-square roughness of the substrate. The latter simulations are still in progress now.

Description of the main results obtained

The carefully prepared systems with the block with long-range elasticity and the flat or rough substrates with several values of fractal dimension and the root-mean-square roughness.

Temperature plots vs. time during preparation of the systems and during approach of the surfaces.

Average pressure vs. distance (time) plots for approach of the block towards the substrate. Comparison of the cases with the flat and self affine fractal substrate surfaces.

The distribution of the perpendicular force acting on atoms of the block in the contact region and the closest separation between the block and the substrate atoms.

The snapshots to control evolution of configurations in time.

Other plots and distributions related to adhesion and friction will be ready after the simulations in progress now will be finished.

Future collaboration with host institution

I have a good and permanent collaboration with Dr. B.N.J. Persson for many years (see Refs. [1-8] and [10-13]). Many of my simulations were performed and our joint publications were prepared during my visits to IFF, FZ-Juelich, Juelich in 2001-2005 (including the present short visit). Dr. B.N.J. Persson also visited me at Moscow State University many times.

So I plan the future collaboration with the host institution IFF, FZ-Juelich and hope that it will be fruitful fot the both sides.

Projected publications/articles to result from the grant

We plan to present results of these calculations at the 4th ESF Nanotribology Workshop to be held June 18-22, 2005 in Porquerolles, France if results are ready before the deadline for the submission of abstracts (for previous presentations see Refs. [10-13]). Also they will be published in one or two joint papers in JCP (similar to results of my previous research visits, see Refs. [1-8]).

Acknowledgments

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Signature: *Dr. V.N.Samoilov, Ph.D.*

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Dr. Vladimir N. Samoilov, Ph.D.
Associate Professor
Department of General Physics
Physics Faculty
Moscow State University
117234 Moscow, Russia
Phone : +7 (095) 9391435 (office)
Phone : +7 (095) 2428828 (home)
Fax : +7 (095) 9391489
E-mail: samoilov@polly.phys.msu.ru