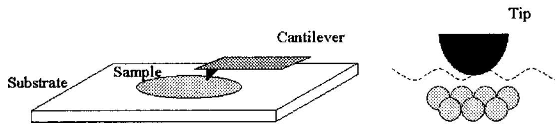

Fig. 1 Schematic of the AFM action

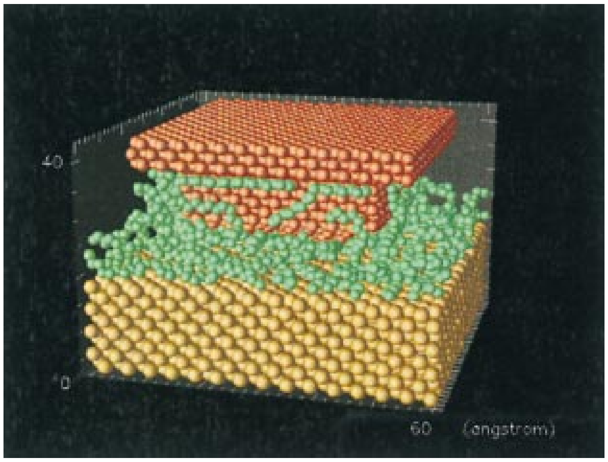

Fig. 2 Instantaneous snapshot of polymer molecular motion

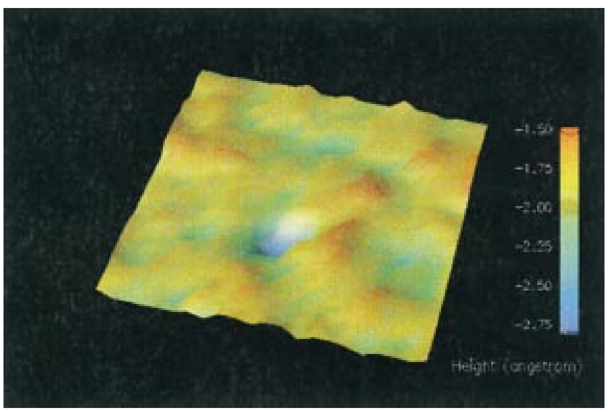

Fig. 3 Topology of the sample surface atomic structure

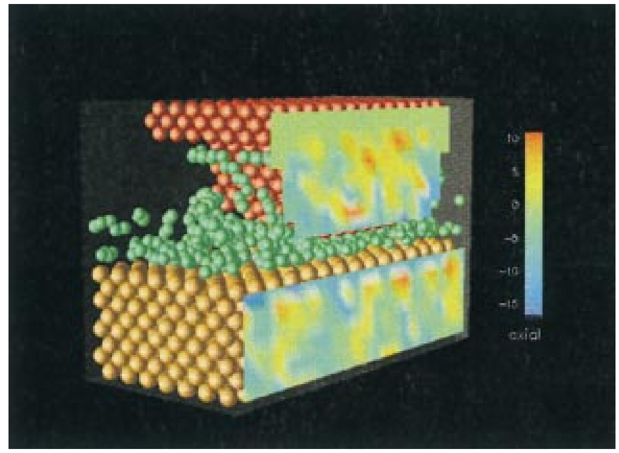

Fig. 4 Image of the atomic normal stress (axial) forces

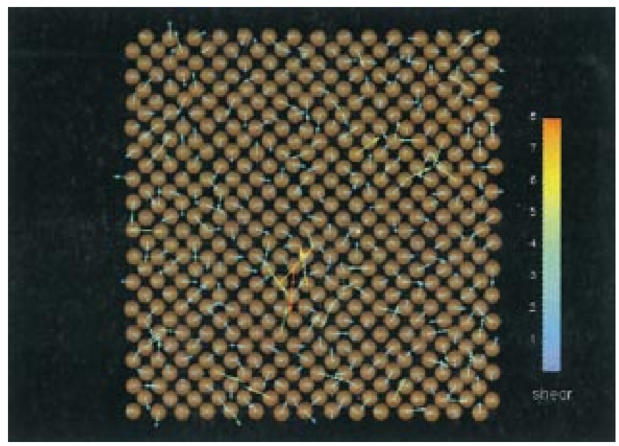

Fig. 5 Image of the atomic shear stress (friction) forces

VISUALIZATION OF ATOMIC FORCE MICROSCOPY FROM MOLECULAR DYNAMICS SIMULATIONS

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A computer visualization method is used to present the details of the imaging action by the surface scanning equipment—Atomic Force Microscope (AFM) from the Molecular Dynamics (MD) simulations. The purpose of the scanning process is to resolve (image) the surface details, to observe the tip-substrate interactions, and to record the dynamics of transport processes in the film down to the atomic or molecular level. The device uses a nondestructive tip to probe the interatomic and intermolecular forces and is schematically shown in Fig. 1. Figures 2 through 5 show results of MD simulations of an AFM cantilever tip that probes a sample covered with the lubricant film. The cantilever tip is made of nickel (Ni, shown in red color), the sample is gold (Au, shown in gold color), and the lubricant film consists of several long chain molecules of the polymer (shown in green color). Figure 2 presents an instantaneous snapshot of the polymer molecular motion around the AFM tip induced by intermolecular interactions between the molecules of the substrate, film, and the cantilever tip. In Fig. 3, we show the topology of the surface atomic structure of the substrate via mapping the local height field by the color image to generate the rubbersheet-like surface. This is virtual representation of the instantaneous topographic image of the surface generated by AFM. Figure 4 presents computer imaging of the short range axial intermolecular forces (i.e., atomic normal stresses) induced by atoms located nearby to the cutting plane, while the atomic level friction forces induced by the tip and polymer molecules on the sample surface are demonstrated in Fig. 5. For the purpose of visualization of the unstructured data irregularly located in space, the mapping surfaces are created to interpolate the scattering data points into correct field values on the mapping surface (Fig. 4).

Acknowledgments

The authors would like to thank Dr. David Luedtke, Professor Uzi Landman from GIT School of Physics, and Dr. William Ribarsky from GIT College of Computing for providing the MD dataset.

