2011

Atomic Friction Studied by Modeling the Buried Inteface

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ABSTRACT

Molecular dynamics simulation is carried out to model the single-asperity friction in atomic force microscope experiments. Superlubricity is achieved through misalignment between the AFM tip and substrate. Direct observation of the buried interface reveals that incommensurability-induced inhomogeneous shear stress can cause ultra-low atomic scale friction.

INTRODUCTION

Atomic friction referring to forces resisting relative sliding at the nanoscale has become increasingly important with the rapid development of micro- and nano-electromechanical systems. The poor understanding and control of atomic friction largely hinders the further miniaturization of mechanical device components. Furthermore, atomic friction is relevant to friction on all length scales because any macroscale contact can be resolved into the sum of its component asperities, where the smallest measurable asperities are at atomic scale. Understanding atomic-scale friction, therefore, has the potential to provide unique insights into larger scale contacts.

The study of atomic friction can benefit greatly from understanding the complex physical processes that occur in the buried interface, the region between the two contacting objects in relative motion.[1-3] Experimental studies of atomic-scale friction are performed primarily using an atomic force microscope (AFM) in which an AFM tip approximating a single asperity is moved laterally across a sample substrate and the resulting friction force is measured. An illustration of a buried interface in AFM experiment is shown in Figure 1. Unfortunately, at this point it is extremely difficult to directly observe nanoscale phenomena within a buried interface during sliding using experimental methods. We turn to molecular dynamics (MD) simulation to investigate the correlation between frictional behavior and the buried interface.

METHODOLOGY

MD simulation is a computational tool used to describe how positions, velocities and orientations of molecules change over time. The simulation is based on a set of equations that describe the interactions between neighboring atoms. These equations relate energy (or force) to the positional configuration of the system, which can, in turn, be used to calculate atom acceleration via Newton's second law. Numerical integration is performed to calculate particle velocities, and then each particle is moved through a distance equal to its velocity multiplied by the simulation time step. The advantage of molecular dynamics simulation is the ability to "see" individual atoms, and we utilize this capability to reveal and understand the details of the tip-substrate interaction in an AFM experiment.

As shown in Figure 1, in a typical experiment, a nanoscale tip attached to an AFM cantilever is dragged to slide against substrate. The force resulting from interaction between the

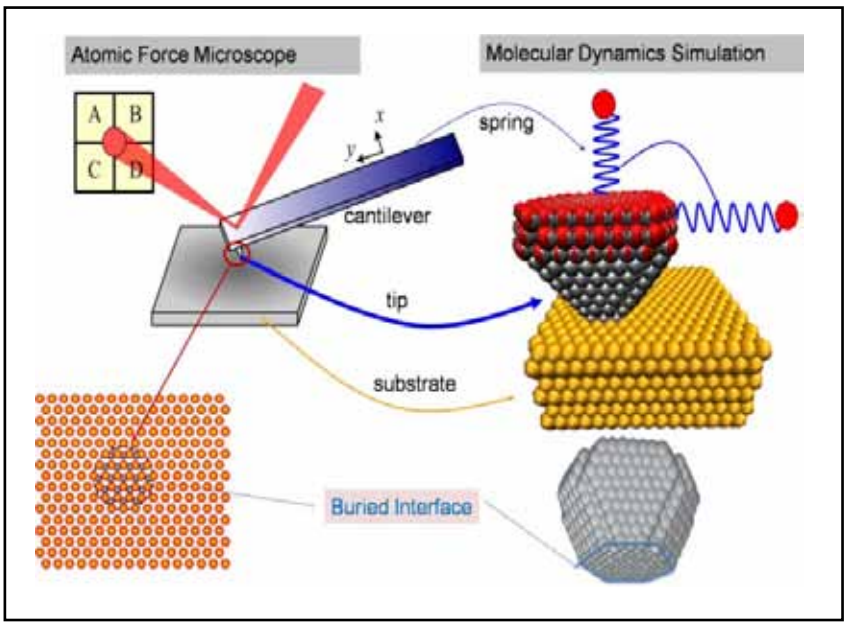

Figure 1 | **Illustration of a molecular dynamics model (*shown on the right*) of an AFM system (*shown on the left*) in which a nanoscale tip attached to a cantilever is dragged to slide against the substrate. The buried interfaces between the tip and substrate are shown below.**

tip and substrate is recorded by measuring the torsion of the cantilever with a laser sensor. In MD simulation, we model the atoms in the apex of the tip and the adjacent substrate. A virtual spring is used to mimic the cantilever to slide the platinum tip (gray) on the gold substrate (yellow) with certain compliance. The atomic interactions are modeled by Embedded Atomic Method (EAM) with Voter-Chen form. The {111} surfaces are chosen as the contact interface, both for the platinum tip and the gold substrate. There is no external normal load (only inter-surface adhesion is considered) and the temperature is maintained at 300 K. The friction force between the tip and substrate are tracked over time. Two representative friction traces are shown in the insets of Figure 2.

RESULTS AND DISCUSSION

Unlike macroscale frictional behavior, which can be well described by a linear relation between friction and normal load, at an atomic level, a variety of parameters can affect the frictional behavior including misalignment between the tip and substrate.

Figure 2 shows the calculated mean friction as a function of the misalignment angle between the tip and substrate. At commensurate angles (i.e., $N{\cdot}60°$, where N is an integer), a very high friction is observed. However, when the rotation angle deviates even a little, the friction drops a few orders of magnitude to almost zero and the system enters the so-called "superlubricity" regime.[4,5] The almost vanishing friction of superlubricity suggests a practical way to control friction at the nanoscale.

To gain a better understanding of the superlubricity phenomenon, we evaluate the shear stress at the buried interface. Figure 3 shows atomic positions (upper) and shear stress distribution (below) at different misalignment degrees. The misalignment angles cause some lattice positions of the tip to coincide exactly with some lattice positions of the substrate. This overlap leads to the development of a superstructure, or Moiré pattern. The misalignment also leads to the inhomogeneous shear stress distribution in the buried interface. Due to the inhomogeneous stress distribution, the negative and positive stresses counteract each other and result in the observed ultra-low friction.

SUMMARY

Superlubricity in atomic friction is achieved through misalignment between the tip and substrate. Direct observation of the buried interface shows that the incommensurability induced inhomogeneous stress is responsible for the vanishing of friction. The manipulation of friction through rotation of the tip and also understanding of its underlying mechanism suggests a practical way to control friction at the atomic level.

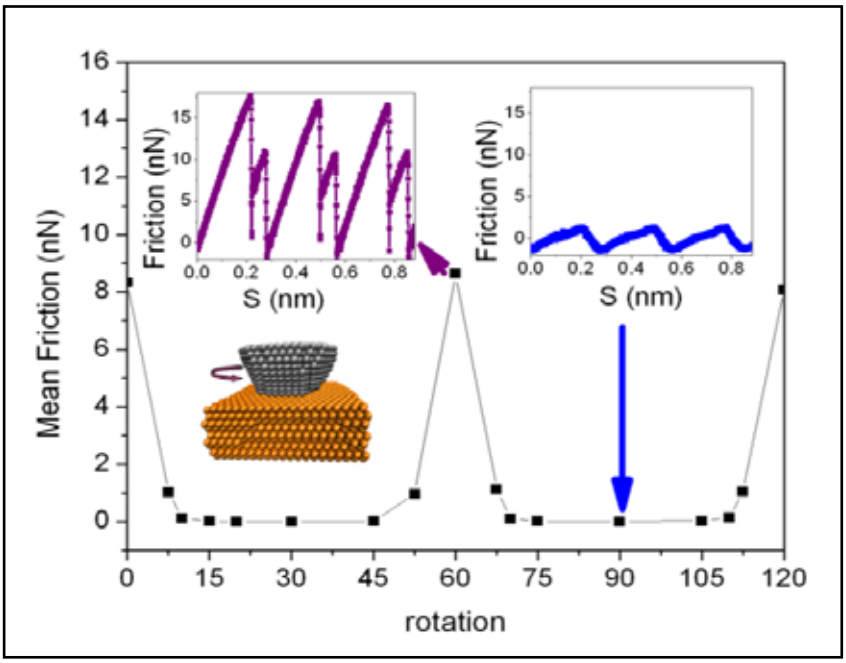

Figure 2 | **Friction as a function of misaligned angle between tip and substrate. Insets are representative force traces at 60° and 90°. Very high friction occurs when the tip and substrate are in registry while superlubricity is observed at other angles.**

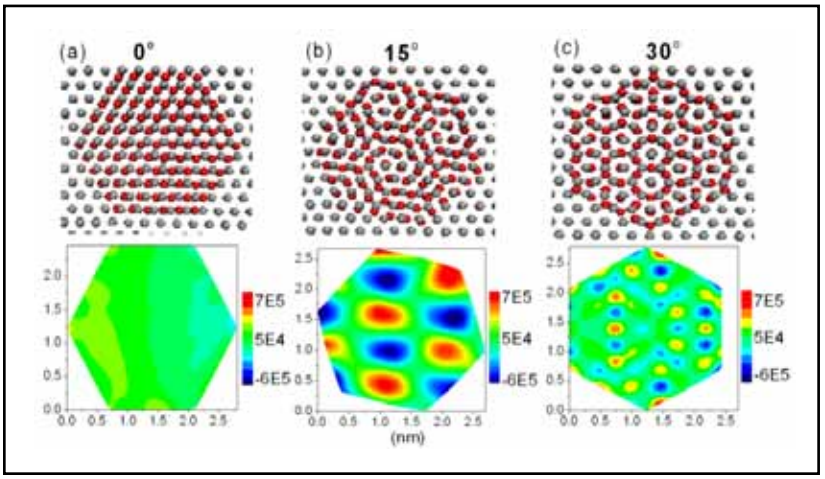

Figure 3 | **Moiré patterns and shear stress distributions resulting from misalignment between tip and substrate. In the upper images, gray circles represent atoms in the top layer of the substrate while red circles are atoms in the bottom layers of the tip.**

ACKNOWLEDGMENTS

This work was done in collaboration with Danny Perez and Arthur F. Voter at Los Alamos National Laboratory (LANL). We are grateful to the National Science Foundation for its support via award CMMI-0758604 and CMMI-0800154.

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