Molecular dynamics simulation of the meniscus formation between two surfaces

Yunfei Chen[a)]
Department of Mechanical Engineering, Southeast University, Nanjing, 210096, People's Republic of China

Jian-gang Weng, Jennifer R. Lukes, Arunava Majumdar, and Chang-Lin Tien
Department of Mechanical Engineering, University of California, Berkeley, California 94720-1740

The molecular dynamics computational method is used to simulate meniscus formation around an asperity in a rough surface represented as a sinusoidal wave. Simulation results show that the meniscus formation depends on the interaction potential between the solid wall and the liquid atoms. For completely and partially dry substrates a meniscus cannot form around an asperity. For partially and completely wetting substrates the asperity helps to adsorb the fluid atoms and form a meniscus. These simulation results confirm that if the film thickness exceeds a critical value, the capillary pressure contributes strongly to stiction. © *2001 American Institute of Physics.*
[DOI: 10.1063/1.1394957]

In ultrahigh recording density disk drives the head and the disk are manufactured with very smooth surfaces (roughness amplitude ~1 nm) and a phenomenon called "stiction" is usually observed. Stiction refers to the high static friction force encountered at the start of operation.[1] Stiction is also encountered in microelectromechanical systems.[2] Many researchers have conducted experiments to study the role of surface roughness, lubricant type, liquid film thickness, and relative humidity on stiction on the head disk interfaces.[3–5] In order to explain the stiction phenomenon two assumptions are proposed. First, it is assumed that the meniscus force causes a steep increase of the contacting load, thus causing increased friction force. A kinetic meniscus model has been proposed by Bhushan[6] to predict the resting stiction force between slider and disk caused by the capillary pressure. This model, however, cannot be used to interpret the meniscus formation on an ultrathin (3–10 nm) film. In this case, the continuous assumption is invalid. It is doubtful that the fluid film can flow as freely as in the bulk state. Another assumption is that it is the attractive forces between the two surfaces and between the surface and the film that cause the increase of the contacting load, thus causing increased friction force. The second model can successfully explain the high friction coefficient but it cannot explain why stiction forces are great enough to pull off the slider.[1] The key problem rests on whether it is possible to form a meniscus around an asperity with an ultrathin film and on the length of time for such meniscus formation. This letter uses molecular dynamics to simulate an ultrathin fluid film confined between two surfaces in order to study the structure and dynamics of the thin film, observe the final film state, and ascertain the possibility of forming a meniscus around an asperity.

Using the Lennard-Jones interatomic potential for argon atoms, the positions of the atoms and the interactive force between the atoms and the surfaces are calculated. The physical model used in the calculation is that of a thin film confined between a smooth surface and a rough surface, as shown in Fig. 1(a). The lower surface is not shown explicitly but is assumed a stationary, smooth surface at $z=0$ to save computation time. The upper wall is thick enough to make it appear infinite to the fluid atoms. Its roughness is represented as a sinusoidal wave surface [Fig. 1(a)]. The surface is described as

$$H(x,y) = A \sin\left(2\pi n \frac{x}{L_x} \right), \qquad (1)$$

where A, n are the wave amplitude and the wave number. L_x is the simulation domain length along the x direction. The Lennard-Jones (LJ) potential[7] represents the interaction between a particle of type A and a particle of type B:

$$V_{AB}(r) = 4e_{AB}\left\{ \left(\frac{\sigma_{AB}}{r} \right)^{12} - \left(\frac{\sigma_{AB}}{r} \right)^{6} \right\}, \qquad (2)$$

where subscripts A, B ($=s, f$) stand for "solid" or "fluid," e_{AB} and σ_{AB} represent the energy and length scale of the potential, and r denotes the distance between the two particles. The lower surface at $z=0$ acts on the fluid atom through a summed LJ potential force. The fluid–solid interactive potential is

$$V_D(z) = \frac{2}{3} \pi \rho_s e_{sf} \left(\frac{\sigma_{sf}}{\sigma_{ff}} \right)^{12} \left\{ \frac{2}{15} \left(\frac{\sigma_{ff}}{z} \right)^{9} - \left(\frac{\sigma_{ff}}{\sigma_{sf}} \right)^{6} \left(\frac{\sigma_{ff}}{z} \right)^{3} \right\} \sigma_{ff}^{3}, \qquad (3)$$

where z is the atom's z axis coordinate. ρ_s denotes the particle density of the lower surface and σ_{sf} is the interactive length scale between the solid atom and the fluid atom, $\sigma_{sf} = 0.941\sigma_{ff}$. Its value is set as close to the mean of σ_{ss} and σ_{ff}. Equation (3) is deduced from Eq. (2) by summing the interactions of a single atom with an infinite smooth surface.

At the initial state the fluid atoms are arranged as a lattice with lattice constant $1.5 \sigma_{ff}$ [Fig. 1(a)]. Periodic boundary conditions are used along the x and y directions. The cutoff radius for r, $r_c = 2.6\sigma$, is introduced to save compu-
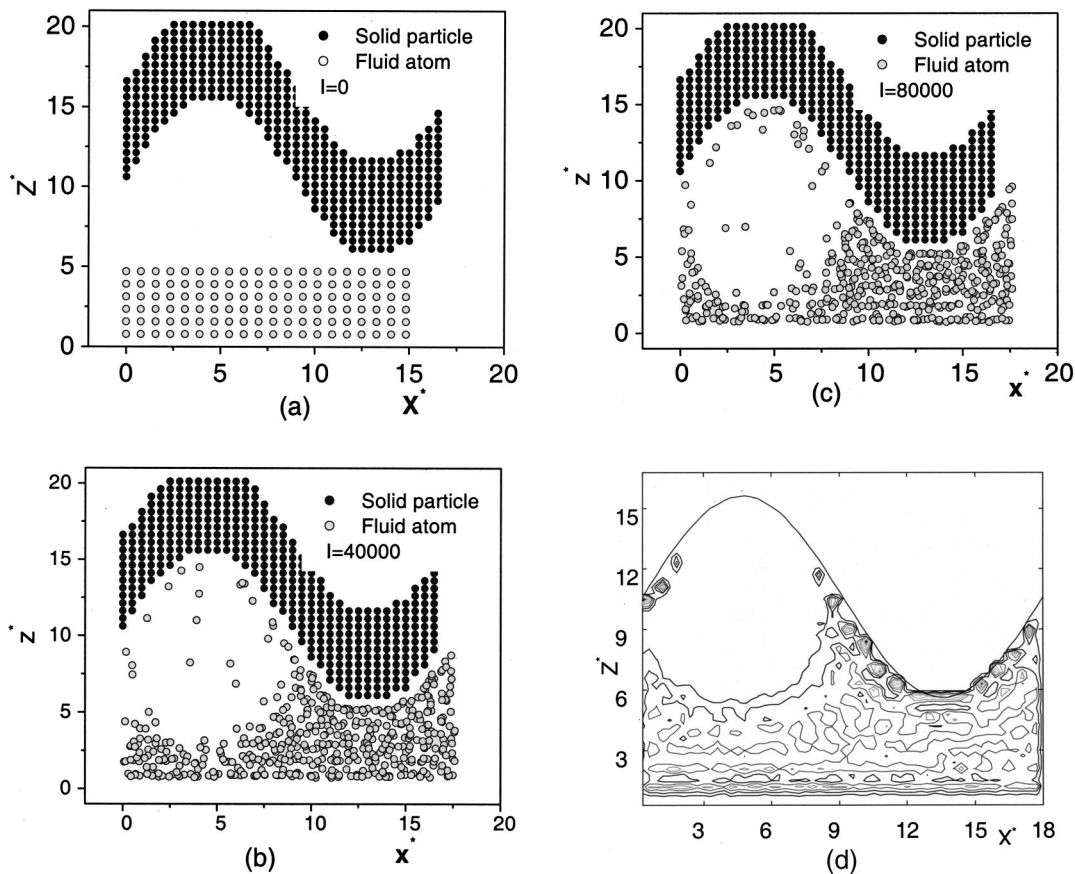
---

a)Electronic mail: yfchen@newton.me.berkeley.edu

FIG. 1. Snapshot of meniscus formation at different time steps. (a) $N=480$ and $I=0$. (b) $N=480$ and $I=40\,000$. (c) $N=480$, $I=80\,000$. (d) Density contour: $N=600$ and $I=80\,000$.

tation time. All quantities with a star superscript are nondimensionalized by the corresponding fluid atom parameter, σ_{ff}, e_{ff}, m_f. The molecules move according to Newton's second law. The velocity Verlet algorithm[8] is used to solve the equations of motion. The time step is set as 5 fs. The fluid atoms are kept at constant temperature $T=99$ K by rescaling the atom velocities every 40 steps. After the initial 20 000 time steps, the positions and the velocities of the fluid atoms are recorded. The equilibrium state is reached after 80 000 time steps.

Figures 1(a)–(c) show the result for the time evolution of liquid meniscus formation. Figure 1(c) gives the final state of the fluid atoms confined between a smooth and a rough surface. During the meniscus formation the atoms at the top
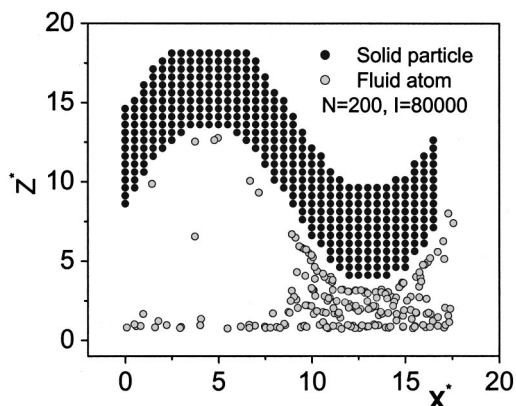
of the fluid move to the asperity first and bridge the upper rough wall with the substrate. When these fluid atoms move a vacancy appears. The neighboring fluid atoms at the top of the layer soon fill the vacancy. This moving and filling procedure occurs during the whole formation process. Through the interaction between neighboring fluid atoms the asperity attracts faraway fluid atoms that are located outside the interaction range for the asperity. More and more fluid atoms move around the asperity until a meniscus is formed. When the top layer of the fluid atoms is exhausted each underlying layer continues this procedure to provide atoms for the meniscus formation. This process can even exhaust the fluid atoms far from the asperity. This differs from the fluid film confined between two smooth surfaces, in which the fluid atoms will distribute over the substrate and the density near the substrate is stable. Also, if the film thickness satisfies the critical condition the film will remain stable.[9,10] When a rough surface moves towards the thin film, as observed from Fig. 1, the fluid atoms will move to the asperity and the thin-film stability is destroyed. This can be further proved in the following simulation. If the liquid film is too thin to bridge the two walls at the initial state, such as $N=200$, $d^*=5.618$, where d^* is the minimum distance between the asperity and the substrate, the meniscus will not be formed. In this case, the liquid atoms are adsorbed to the substrate and after 80 000 time steps no meniscus is found, and the film keeps stable. If the displacement between the two walls is decreased from $d^*=5.618$ to $d^*=3.618$, a meniscus will form after 80 000 time steps, as shown in Fig. 2.
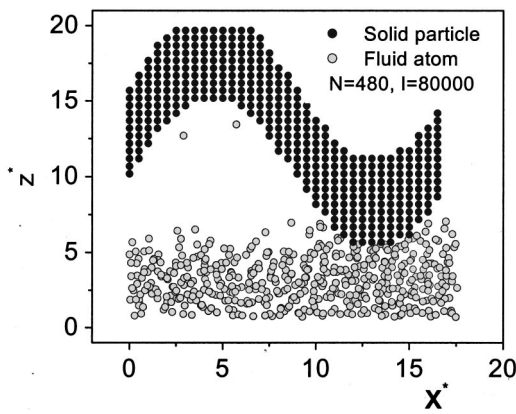

FIG. 2. Meniscus formation for a small number of atoms $d^*=3.618$.

FIG. 3. Fluid atoms confined between partially drying solid walls ($\varepsilon_r = 0.4$).

Once the meniscus is formed, the shape of the meniscus remains stable, depending only on the interactive potential between the solid wall and the liquid atoms. The meniscus shape can be measured by the contact angle, which can be obtained from a visual inspection of the two-dimensional density contour for the meniscus.[7] Figure 1(d) gives such a density contour. At different time steps after equilibrium the contact angle remains constant. On the other hand, if the interactive potential between the solid wall and the fluid atoms is decreased from a partially wetting state to a partially drying state, a meniscus cannot form ever for a large number of atoms. The fluid film will distribute over the substrate, as shown in Fig. 3. The attractive force acting on the upper solid wall by the fluid atoms depends on the interaction potential between the wall and the fluid atoms. Figure 4 gives
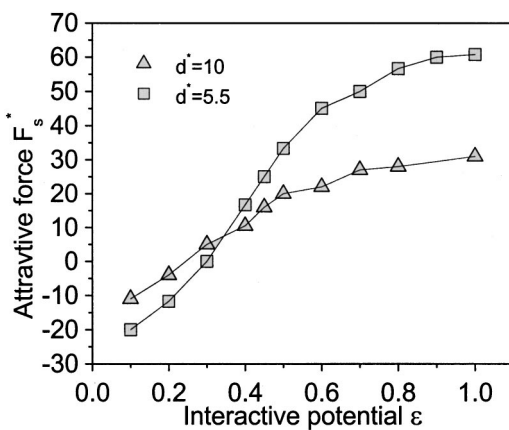
the nondimensional attractive force, F_s^*, versus the interaction potential parameter:

$$F_s^* = \frac{F}{R^*} \frac{\sigma_{ff}}{e_{ff}}, \tag{4}$$

where F, R^* are the attractive force acted on the upper solid surface and the radius of meniscus, respectively. A meniscus cannot form between $\varepsilon_r = 0.1 - 0.4$, so the attractive force increases almost linearly with the interactive potential. Between $\varepsilon_r = 0.4 - 0.55$ the attractive force gets a sharp increase, which means more fluid atoms concentrate on the upper solid wall. With $\varepsilon_r > 0.55$ and for a fixed number of atoms the attractive force will increase slowly.

In conclusion, the formation procedure of a meniscus around an asperity has been simulated. The simulation results show that the meniscus formation only depends on the interaction potential between the solid wall and the fluid atoms. For a partially drying wall it is impossible to form a meniscus. For partially and for completely wetting walls the initial separation between the solid wall and the fluid atoms will affect the formation time. The driving force to form a meniscus is the interaction force between the solid wall and the fluid particles. Even for an ultrathin (1 nm) liquid film, a meniscus can form around a partially or completely wetting asperity. Although the asperity does not directly act on the faraway fluid atoms, it indirectly attracts these atoms to form a meniscus through the interaction of neighboring fluid atoms. The formation time only depends on the interaction force and the initial space between the solid wall and the fluid atoms. Increasing the liquid film thickness induces a high attractive force after meniscus formation, causing a high friction force.

FIG. 4. Attractive force between the fluid atoms and the upper solid wall.

[1] B. Bhushan, *Tribology and Mechanics of Magnetic Storage Devices* (Springer, New York, 1990).
[2] R. Maboudian and R. T. Howe, J. Vac. Sci. Technol. B **15**, 1 (1997).
[3] C. Gao and B. Bhushan, Wear **38**, 201 (1995).
[4] J. L. Streator, B. Bhushan, and D. B. Bogy, J. Tribol. **113**, 21 (1991).
[5] S. Wang and K. Komvoupolous, J. Tribol. **122**, 246 (2000).
[6] B. Bhushan, C. A. Kotwal, and S. K. Chilamakuri, J. Tribol. **120**, 42 (1998).
[7] M. J. P. Nijmeijer, C. Bruin, and A. F. Bakker, Phys. Rev. A **42**, 6052 (1990).
[8] W. C. Swope, H. C. Andersen, P. H. Berens, and K. R. Wilson, J. Chem. Phys. **76**, 637 (1982).
[9] J. Koplik and J. R. Banavar, Phys. Rev. Lett. **84**, 4401 (2000).
[10] R. Khanna and A. Sharma, J. Colloid Interface Sci. **195**, 42 (1997).