

Molecular dynamics (MD) studies on Friction Anisotropy at Ni(100)/(100) interface

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Abstract:

The origin of friction comes from the atomic interaction at interfaces. Analytic theories indicated that there is no static friction on clean incommensurate interfaces, while a recent experiment revealed that the static friction coefficient was anisotropic with respect to the lattice orientation, but did not vanish on two clean Ni(100) mis-orientated surfaces. To understand this friction anisotropy and the difference between theory and experiment, we carried out a series of Non Equilibrium Molecular Dynamics (NEMD) simulations for sliding of Ni(100)/Ni(100) interfaces under a constant force(see figure 1). We found that the clean, flat, and incommensurate interface indeed has a very small static friction coefficient. However, surface roughness can increase the static friction on the incommensurate interfaces dramatically and increase, to a lesser extent, the friction on the commensurate interfaces. Thus, the rough surfaces show similar anisotropy behavior as experimental results. The dynamic frictional coefficients are comparable to the

experimental values as that observed in experiments for the $\theta=0^\circ$ and the $\theta=45^\circ$ orientated interfaces, and show the same anisotropic behavior.

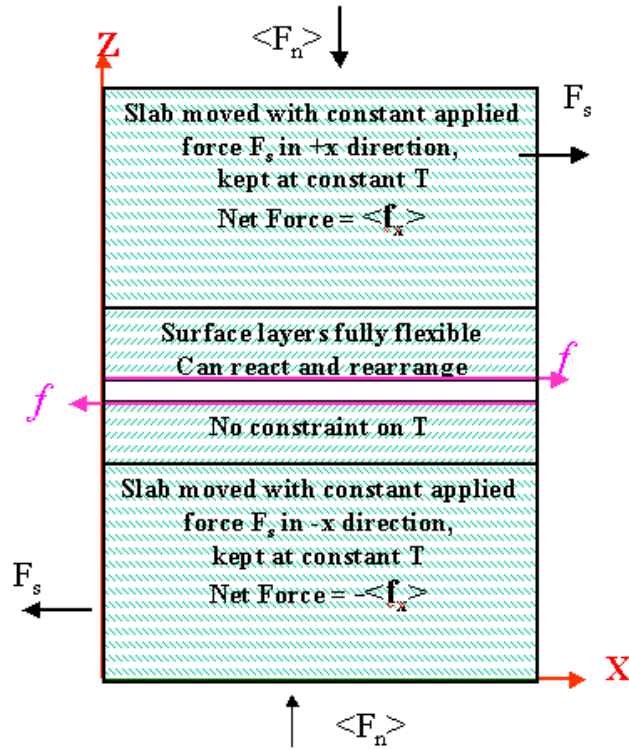


Figure 1 Projection along y direction of a 2D periodic (along x and y directions) cell for Tribosimulations (steady state nonequilibrium molecular dynamics). F_s is the applied external force on two moving slabs with 6 layers of atoms. f is the frictional force during the sliding of two slabs, and $\langle F_n \rangle$ is the normal load on z direction. The static frictional coefficient defined as the ratio of F_s , the force needed to initiate motion between objects at rest, and the load $\langle F_n \rangle$. And the dynamic frictional coefficient can be calculated from the ratio of f and $\langle F_n \rangle$.

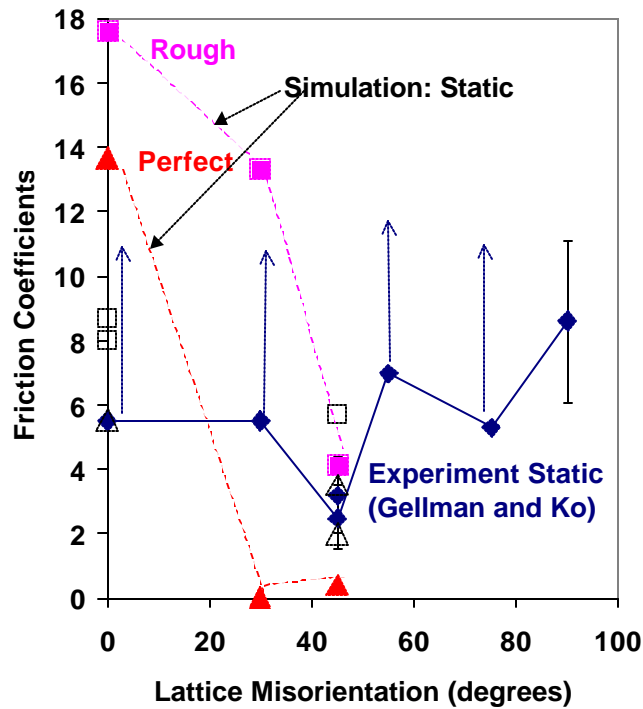


Figure 2 Friction coefficient as a function of the lattice misorientation angle between two Ni(100) surfaces. Solid diamonds are the experimental static friction coefficients measured by Gellman and Ko, the point and upward arrows represent the lower limit of the values. The solid symbols are static friction coefficients from simulation, and open symbols are dynamic friction coefficients. Squire patterns are for flat interface and triangles are for rough interface.

Acknowledgments

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