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Molecular dynamics studies of friction between bare and oxidized silicon surfaces WOO KYUN KIM, MICHAEL FALK, The University of Michigan — Using molecular dynamics simulation we examine the friction between a bare silicon tip and a silicon surface under perfect vacuum conditions. The simulations utilize a Stillinger-Weber model for the Si-Si interactions. In the case of bare silicon (100) the proper surface reconstructed is verified. Silicon-silicon sliding leads to high friction and significant wear due to the strong adhesive force between tip and surface. Repeated adhesion and shearing produces a stick-slip motion. The quantity of material lost during sliding depends on the relative orientation of the dimer rows between the reconstructed surfaces of the tip and substrate. Little dependence on the temperature or the normal force is observed in this case. The frictional force does not change significantly even when an upward normal force is applied to the tip force, although the quantity of lost material depends on the magnitude of upward normal force. The geometry and elasticity dependence of the stick-slip motion has also been analyzed. We have also begun investigations of a similar geometry in which the silicon is coated with a thin oxide layer. A charge transfer potential having 3-body terms as well as pair-wise interactions is being used to model the amorphous silica interactions. These simulation results will be compared to the recent AFM experiments by Schirmeisen et al. measuring the frictional forces between an oxidized silicon tip and substrate.

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