Molecular Dynamics Simulations of Sliding Friction on Diamond Surfaces

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Abstract

Diamond (001) surface has been constructed and investigated using both quantum mechanics (QM) calculation and Molecular Dynamics (MD) simulations. We studied the binding energies for different adsorbates with different coverage and built the surface accordingly. With the MD method, we carried out sliding friction simulations for the following systems: 1) 100% coverage H-terminated diamond (001)(2×1) surface; 2) 100% coverage OH- terminated diamond (001)(2×1) surface; 3) 100% coverage O-terminated diamond (001)(1×1) surface; 4) 50% coverage SH-terminated diamond (001)(2×1) surface; 5) 100% coverage CH$_3$-terminated diamond (001)(2×1) surface. Simulation results showed that OH-, O- and CH$_3$-terminated surfaces have low friction, H-terminated surface has relatively high friction and SH-terminated surface has high friction. To study the influence of the adsorbates coverage on the friction, we also did the sliding simulation for 50% coverage OH-terminated diamond (001) surface. The friction coefficient for 50% coverage OH-terminated surface is much higher than that of 100% coverage OH surface and in a same magnitude as that of 50% coverage SH-terminated surface, implying that the coverage of adsorbates may be the reason for high friction of SH-terminated surface. Decreasing of adsorbates coverage changes the surface potential profile, leading to the increase of frictional force. The relative high friction for H-terminated surface is due to the high damping constant of H-terminated surface.

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