Effects of atomic-scale roughness on adhesion between diamond surfaces

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CNST Project Leader Rachel Cannara and collaborators from the United States Naval Academy (USNA) and the University of Pennsylvania have shown that atomic-scale surface roughness has a strong influence on adhesion for diamond, amorphous carbon, and model diamond nanocomposites.

Using atomic force microscope (AFM) measurements performed at the University of Wisconsin-Madison, molecular dynamics (MD) simulations, and ab initio density functional theory (DFT), they investigated the adhesive physics and mechanics of nanoscale interfaces between diamond surfaces.

For atomically smooth surfaces, the greater density of atoms in the (111) plane would be expected to lead to a higher electrostatic dipole moment per unit area and a higher work of adhesion than the (001) orientation. However, the AFM measurements, supported by detailed simulations of model diamond nanocomposites, challenge this assumption in a way that can only be explained by variations in atomic-level surface roughness, which for single crystals can arise from orientation-dependent growth mechanisms.

Unlike previous ab initio studies that compared surface energies for diamond (111)(1×1)-H surfaces and unreconstructed diamond (001)(1×1)-H surfaces, the MD simulations performed at USNA simulate the (2×1)-reconstructed C(001)-H surface. The simulations predict that the C(001)(2x1)-H surface is energetically favorable to the

unreconstructed surface. Corroborating these simulations, high-precision AFM lateral force images of the (001) surface revealed (2×1) dimer-row domains.

In addition to using the appropriate (001) surface structure, the MD simulations account for long-range van der Waals interactions, as well as surface energies, when calculating the work of adhesion for each interface. Moreover, the ab initio DFT calculations reveal the presence of bond dipoles on single-crystal diamond surfaces.

Using AFM, the contact mechanics of the interface was extracted from the load-dependence of the contact area during sliding friction experiments. Works of adhesion were then calculated from the appropriate contact mechanics model and from pull-off forces measured during the sliding experiments and quasistatic force-displacement measurements. These results have broad implications for the design of MEMS/NEMS devices that incorporate diamond or diamond-like materials.

More information: Atomistic Factors Governing Adhesion Between Diamond, Amorphous Carbon, and Model Diamond Nanocomposite Surfaces, P. L. Piotrowski, et al. *Journal of Adhesion Science and Technology* 24, 2471 - 2498 (2010). www.ingentaconnect.com/content … 24/F0020015/art00010

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