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Adhesion in Silicon Diamond Nanocontacts is Boosted by Covalent Bonding and Atomic-Level Plasticity

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Opinion

Nano indentation and sliding studies were carried out in situ using a transmission electron microscope employing single-crystal silicon atomic force microscope probes in contact with diamond surfaces in vacuum. The experimentally measured works of adhesion after sliding were much higher than the values expected for pure van der Waals interactions. Furthermore, during the sliding, the works of adhesion increased with both normal stress and speed, demonstrating that applied stress played a key part in the interface's response. Complementary Molecular Dynamics (MD) simulations were performed to shed light on the atomic-level events that took place throughout the investigations. Two important phenomena were proven in simulations employing crystalline silicon tips with variable degrees of roughness and diamond substrates with varying quantities of hydrogen termination. Covalent bonds formed across the interface first, with the amount of bonds produced influenced by the substrate's hydrogen termination, tip roughness, applied stress, and the stochastic character of bond formation. Second, for initially rough tips, sliding motion and the application of shear stress resulted in an increase in irreversible atomic-scale plasticity, which tended to smoothen the tips' surfaces, resulting in an increase in adhesion. Sliding, on the other hand, roughened some of the initially smooth points. The empirically determined works of adhesion match the intrinsic van der Waals work of adhesion for an atomically smooth silicon diamond contact obtained from MD simulations in the limit of low applied stress. The findings offer mechanistic explanations of sliding-induced alterations of interfacial adhesion, which could be useful in applications involving adhesive interfaces that are exposed to sliding to applied shear forces and displacements.

Tribological phenomena such as friction, wear, lubrication, and adhesion pervade everyday life and have a large economic influence in industry and research. Silicon and diamond are two essential materials in tribology, especially in small-scale applications. In the semiconductor and Micro Electromechanical Systems (MEMS) industries, silicon is the most commonly used material. Silicon offers potential for application in MEMS; however, because to reliability concerns arising from adhesion, friction, and wear challenges, only a few MEMS devices exploiting contacting surfaces have been commercialised. The development of reliable MEMS devices that require contacting surfaces during their manufacture or operation, such as the digital mirror device and MEMS switches, has necessitated proper tribological engineering that takes stickiness into account. Diamond is the hardest substance known to man, with extremely minimal friction and wear. As a result, diamond is a vital material to research for applications that require great strength and wear resistance, such as machining tools, mechanical seals, MEMS switches, and AFM probes. In these applications, as well as in the precision manufacture of silicon-based products utilising diamond tools, contact between diamond and silicon can occur. In this paper, we present the findings of in situ Transmission Electron Microscope (TEM) Nano indentation tests of silicon Nano asperities sliding on a flat diamond surface. After sliding the Nano asperity along the surface at a specified normal load and speed, adhesion is measured. The usual contact stress and sliding speed are found to have a significant impact on the measured adhesion. MD simulations of silicon probes with varied degrees of roughness in normal and sliding contact with diamond surfaces provide atomic-level insight into the adhesion, plasticity, and tribochemistry that is presumably occurring in the experimental research.

Overall, the MD simulations show that tip sample covalent bonding is a plausible mechanism for explaining the experimental result of adhesion values over the van der Waals limit, with a wide range of values. However, the magnitudes of the adhesion increases seen in simulations are not as significant as they are in tests. There are some significant differences between the simulations and the experiments that may explain why the simulations do not capture the same degree of covalent bond formation as the observations. For starters, the lifetime of trials is many orders of magnitude longer than simulations. Due to processing constraints, simulations are limited to less than a millisecond. The time duration of the experiments/simulations is important since covalent bonding is a stochastic process that requires enough elapsed time to have a statistically significant

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impact. Second, the roughness, hydrogen termination, and tip size of the contacting surfaces all have a role in the creation of interfacial bonds during the sliding process. The exact atomic-scale nature of the surfaces utilised in the tests cannot be determined. Third, the number of interfacial covalent bonds existing at the point of tip retraction is affected by sliding distance and sliding speed. The MD sliding speeds must be several orders of magnitude quicker than in experiments due to computational constraints. The experimental methods utilised in this work is incapable of obtaining the speeds used in simulations, which are on the order of metres per second. It is not advisable to extrapolate from simulation results to conclusions about the speed dependency of covalent bonding in experiments since it is completely plausible that such high speeds may sample a different regime of the speed-dependence of adhesion. Furthermore, and probably more importantly, experimental speeds were varied over a two-order-of-magnitude range, which is far greater than the relative speed variation evaluated in the simulations. Given the tiny number of interfacial connections produced during sliding, the range of speeds explored in the simulations is unlikely to be large enough to detect any consistent adhesion trends.