Atomic–scale Processes in Adhesion and Wear Elucidated by *In Situ* TEM Tribological Studies and Atomistic Modeling

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1. Introduction

As technology scales shrink to nanometer length scales, tribological interactionsplay an increasingly dominant role in the physics of contact. For example, tip-based data storage, nanomanufacturing, and nano-electromechanical systems rely on knowledge and control of adhesion, friction, and wearat nanoscale contacts. A lack of fundamental insight hinders the advancement of these technologies. We will discuss the application of *in situ* experimental methods in combination with atomistic theories and simulations to develop new, physically-based insights into adhesion and wear at nanoscale contacts.

2. Effect of roughness in nanoscale adhesion

Surface roughness is known to affect adhesion at macroscopic scales. However, the atomic-scale roughness of tips used in scanning probe microscopy (SPM) is rarely measured or accounted for. We characterized the atomic-scale roughness of carbon-based SPM probes, and measured the corresponding effect on adhesion using simulations and experimental techniques[1].

Adhesion tests were conducted inside of a transmission electron microscope (TEM), using a modified *in situ* nanoindentation apparatus. Nanoscale asperities composed of either diamond-like carbon (DLC) or ultrananocrystalline diamond (UNCD) were brought into contact with a flat diamond substrate.Sub-nanoscale roughness was characterized *in situ* immediately before and after contact. Complementary adhesion simulations were conducted using molecular dynamics (MD).Over the range of roughness tested, the work of adhesion decreased by more than an order of magnitude as roughness increased, with a consistent trend observed between experiments and simulations. The dependence of adhesion on roughness was accurately described by a simple analytical model.

This combination of simulation and *in situ* experimentation allowed exploration of an unprecedented range of tip sizes and roughness length scales. The results indicate that present approaches for measuring work of adhesion values contain significant uncertainty due to atomic-scale roughness.

3. Wear as a stress-assisted chemical reaction

We will then discuss new insights into nanoscale wear[2]. We show that ultrastrong materials can be used to be greatly reduce nanoscale wear[3-5]. We then demonstrate the ability to characterize single-asperity wear with high precision by *in-situ*TEM wear tests.Silicon probes were worn against a flat diamond substrate.The volume loss due to wear is well-described as atom-by-atom removal, modeled usingstress-assisted chemical reaction kinetics[6]. We resolve worn volumes as small as 25±5 nm^3. The rate of atom removal depends exponentially onstress in the contact, as predicted by chemical rate kinetics.Activation parameters are consistent with an atom-by-atom process. These results establish atomic attrition as the primary wear mechanism of silicon at low loadsthrough direct observation.

4. References

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