Friction and fracture of 2D materials

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ABSTRACT

Interfacial strength and surface damage of single- and multi-layer hexagonal boron nitride (h-BN), molybdenum disulfide (MoS_2), and graphene films were studied via atomic force microscopy-based progressive-force and constant-force scratch tests and Raman spectroscopy. The results showed that single-layer h-BN, MoS_2, and graphene strongly adhere to the SiO_2 substrate, which significantly improves its tribological performance. Moreover, defect formation from scratch testing was found to affect the topography and friction force differently prior to the failure, which points to distinct surface damage characteristics. Interestingly, the residual strains at scratched areas suggest the scratch test-induced in-plane compressive strains were dominant over tensile strains, thereby leading to buckling in front of the scratching tip and eventually failure. As the number of layers increased, the tribological performance of atomically-thin h-BN, MoS_2, and graphene were found to significantly improve due to an increase in the interfacial strengths and a decrease in the surface damage and friction force.

KEYWORDS

Interfacial strength, surface damage, two-dimensional materials, atomic force microscopy

INTRODUCTION

Two-dimensional (2D) materials such as single- and multi-layer h-BN, MoS_2, and graphene have attracted intensive interest due to their remarkable frictional properties, with coefficients of friction from 0.001 to 0.1.[1-3] Although initial studies have demonstrated the potential of these materials in greatly reducing friction and wear in mechanical systems,[1,2] the surface damage characteristics of atomically-thin h-BN, MoS_2, and graphene specimens have not been fully investigated. In this study, the film-to-substrate interfacial strengths and surface damage of atomically-thin h-BN, MoS_2, and graphene were studied using atomic force microscopy (AFM) progressive-force and constant-force scratch tests. Based on the progressive-force scratch tests, interfacial strengths for single-layer h-BN, MoS_2, and graphene were evaluated from critical forces, which demonstrated that these atomically-thin materials strongly adhere to SiO_2. The constant-force tests showed the evolution of damage as a function of normal force and revealed distinctive surface damage characteristics. The residual in-plane compressive strains at scratched areas suggested a general failure mechanism in 2D materials.[3]

EXPERIMENTAL/THEORETICAL STUDY

Single- and multi-layer h-BN, MoS_2, and graphene specimens were produced from high-quality single-crystal h-BN, MoS_2, and graphite via micro-mechanical exfoliation. The exfoliated materials were gently pressed against and transferred to an Si wafer capped with a 300-nm thick SiO_2 layer. A nanocrystalline diamond AFM tip with a tip radius of 40 nm was used in both the progressive-force and constant-force tests. In the progressive-force tests, specimens were scratched under a progressive normal force for one scratch line with the distance of 2 μm; the normal force increased from 400 nN to 4000 nN to find the critical force. In the constant-force tests, specimens were scratched in a defined area of 1 μm × 1 μm under constant normal force; the normal forces ranged from 500 nN to 5000 nN to observe surface damage evolution. After the scratch tests, topography and frictional behaviors of the scratched areas were studied via intermittent-contact mode and contact mode AFM and Raman.

RESULTS AND DISCUSSION

The friction force variation with respect to normal force during the progressive-force scratch tests was monitored as shown in Figure 1(a), and the critical force was characterized by the normal load at which there was an abrupt increase in friction force. Scratch tracks were observed in the subsequent topographic and friction force microscopy (FFM) images as shown in Figures 1(b) and 1(c). Based on these observations, the critical forces for single-layer h-BN, MoS_2, and graphene were 900 ± 200 nN, 1300 ± 150 nN, and 3300 nN ± 200 nN, respectively. From the topographic images, single-layer h-BN and MoS_2 were found to tear off and expose the substrate, shortly after scratch tracks were observed. The scratch tracks exhibited an increase in friction just prior to the failure, which indicates that defects were likely formed. Interestingly, in the case of single-layer graphene, a height decrease was observed prior to failure. However, FFM showed that the scratch tracks maintained their low frictional behavior. This suggests that the substrate was plastically deformed, but given the superior mechanical strength of graphene, the film remained intact to failure.[3]

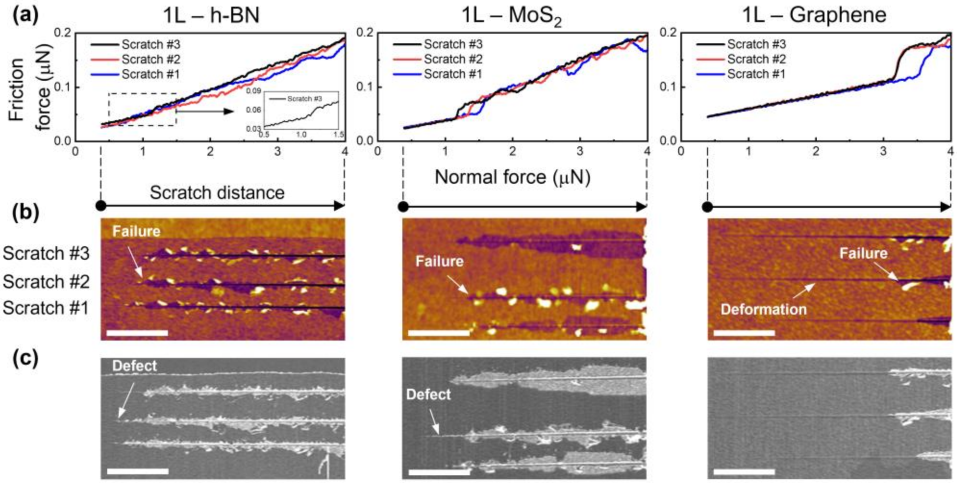

Fig. 1. Progressive-force scratch tests for single-layer h-BN, MoS_2, and graphene. (a) Friction force variation with normal force. (b) Topographic and (c) FFM images of scratch tracks. In (b) and (c), the scale bars are 500 nm.[3]

In the constant-force scratch tests, single-layer h-BN failed at 1500 nN normal force. Shortly before failure, a height decrease of about 0.3 nm was observed, while its friction force was constant. Raman spectra showed the E_{2g} frequency at scratched areas increased by 0.3 cm^{-1} to 0.8 cm^{-1} as compared to as-exfoliated specimens, which suggests in-plane compressive strain. As normal force increased, the blueshift of the E_{2g} peak was constant, which implied that the amount of compressive strain was also constant. For single-layer MoS_2, complete failure was observed at 2000 nN normal force, with the removal of the film from the substrate. Raman spectra showed decreases in intensity and increases in frequency for the E_{2g}^{1} and A_{1g} peaks at 2000 nN, which was attributed to in-plane and out-of-plane compressive strains (smaller normal forces did not exhibit these changes). For single-layer graphene, a height decrease of 1.6 nm was observed prior to failure at 5000 nN. No changes in friction behavior were observed at scratched areas. Raman spectra exhibited changes to the 2D and D intensities and G frequency, which were accredited to defect formation and in-plane compressive strain.[3]

CONCLUSION

The results suggest three stages in the evolution of surface damage. At low normal force, no change in topography and friction force was observed, which points to elastic deformation in the scratched area. As normal force increased, the formation of defects in the film and plastic deformation in the substrate were noted. At the critical force, delamination of the film occurred. The compressive strain-induced buckling in front of the tip was the primary source of mechanical instability in 2D materials.

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