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Molecular dynamics study on friction of multigrain graphene ADITYA KAVALUR, WOO KYUN KIM, Univ of Cincinnati — In addition to its extraordinary mechanical, electronic, and chemical properties, graphene is also a promising material for solid lubrication, which can be used for both macroscopic and small-length scale devices such as MEMS/NEMS. Although a significant number of research efforts have been devoted to unveiling the physical origin of its tribological properties from both experimental and theoretical standpoints, there are still many phenomena which remain far from completely understood. Graphene synthesized by CVD (chemical vapor deposition) is featured with the multi-grain structure, which may have detrimental effects on its mechanical and tribological properties. However, the friction of polycrystalline graphene has rarely been studied. In this study, we investigate the tribological properties of polycrystalline graphene using molecular dynamics methodology. Multigrain structures are created using a novel method and tested against pristine substrates (P-M), these results are compared with pristine-pristine (P-P) interactions. The P-M models exhibit a lower and wider range of friction forces, which may be explained through their individual configurations and a novel orientation-dependent mechanism of friction.

Aditya Kavalur
Univ of Cincinnati

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