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Atomistic Simulation Studies on the Friction of 2D materials MINWOONG JOE, CHANGGU LEE, Department of Mechanical Engineering and Center for Human Interface Nano Technology (HINT), Sungkyunkwan University — Frictional properties of two-dimensional (2D) layerd materials including graphene, MoS_2, $NbSe_2$, and h-BN, have been revealed using atomic force microscopy (AFM) [1]. All the materials exhibit similar trends on friction: the thicker the sheet the lower the friction is. Puckering effect has been suggested as the primary mechanical reason for this thickness-dependent behaviors. Despite this novel findings, detailed atomic-scale processes during tip sliding against such atomically thin sheets are not fully understood yet. In this work, we provide a detailed study of the role of the buried interface between tip and surface on atomic friction using molecular dynamics (MD) simulation. We investigate the magnitude of puckering under various tip and surface conditions such as tip size and surface orientation, to unravel its effect on friction. Our systematic approach could provide a comprehensive understanding of friction phenomena at atomic level.

[1] C. Lee et al. *Science* **328** (2010) 76

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