

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Interlayer Mechanics of Commensurate Boron Nitride Nanotubes**

HOMIN SHIN, KEUN SU KIM, BENOIT SIMARD, DENNIS KLUG, National Research Council Canada — While two-dimensional van der Waals (vdW) layered materials (e.g., graphite or hexagonal boron nitride) have long been recognized as low-friction solid lubricants, a recent experiment reported that multi-walled boron nitride nanotubes (BNNTs) exhibited ultrahigh interlayer friction in contrast to the superlubric sliding behavior of multi-walled carbon nanotubes (CNTs). Given the similarity in their crystallographic structures, these observations raise fundamental questions regarding the origins of friction and energy dissipation in highly confined geometries. Using vdW modified density functional theory (DFT) we investigate the mechanism of the strong mechanical coupling between two concentric layers of commensurate BNNTs. Our findings provide new insights into atomic-scale interlayer friction that will be important for the development of nanodevices or nanocomposites based on BNNTs and CNTs.

Homin Shin  
National Research Council Canada

Date submitted: 11 Nov 2016

Electronic form version 1.4