Supplementary information

Molecular dynamics simulations of nanoscale and sub-nanoscale friction behavior between graphene and a silicon tip: analysis of tip apex motion

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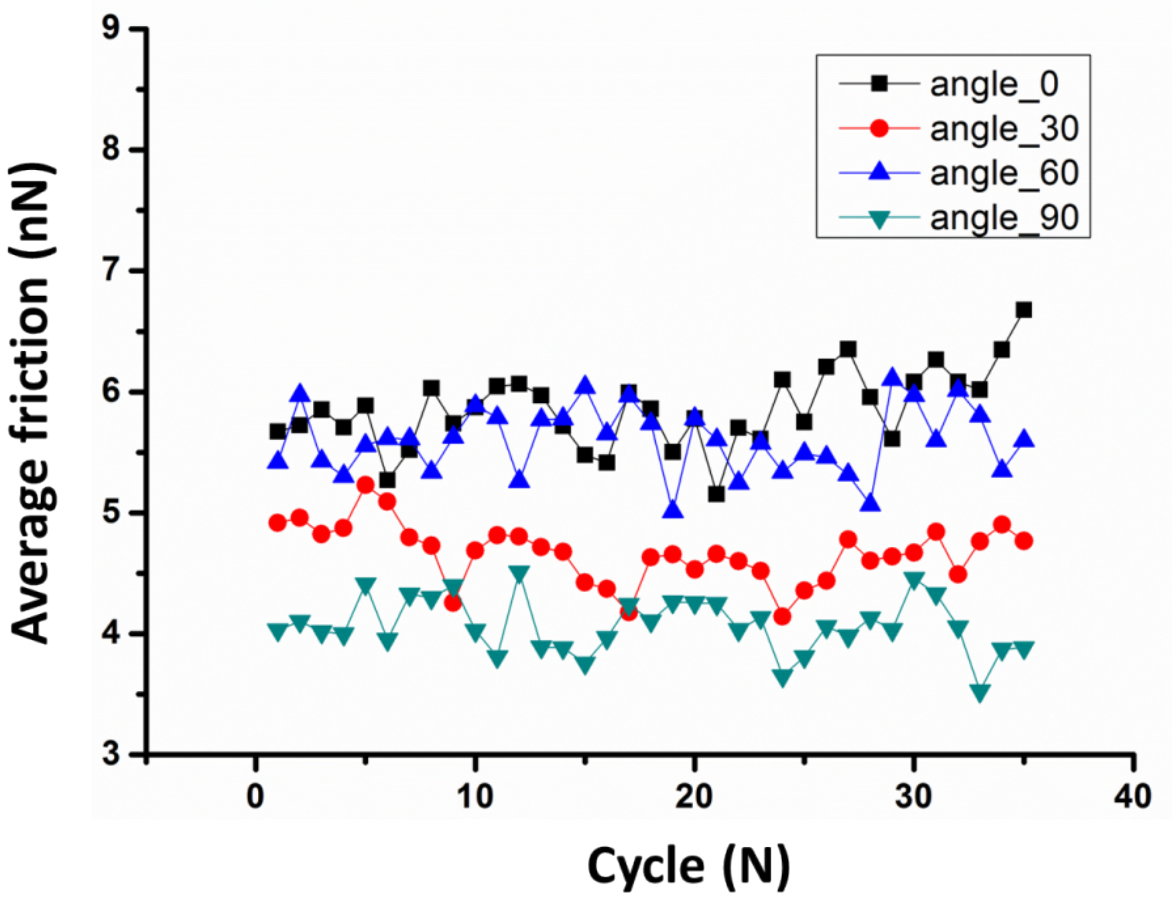

Figure S1. Average friction of different scan direction in FFM experiment for 35 cycles. frictions maintain constant values with the fluctuation of 1nN. This implies that the oxidation has not been significantly occurred in the FFM experiment.

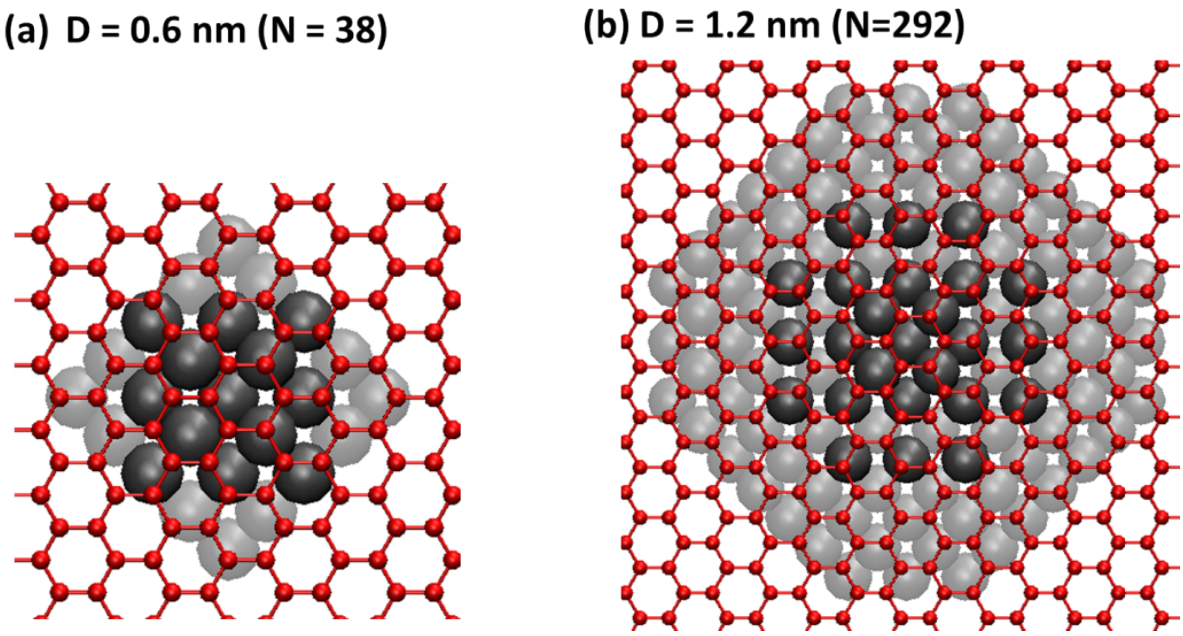

Figure S2. Contact area is defined with the first and second nearest layer of silicon tip. Dark gray atoms represent silicon atoms in contact area.

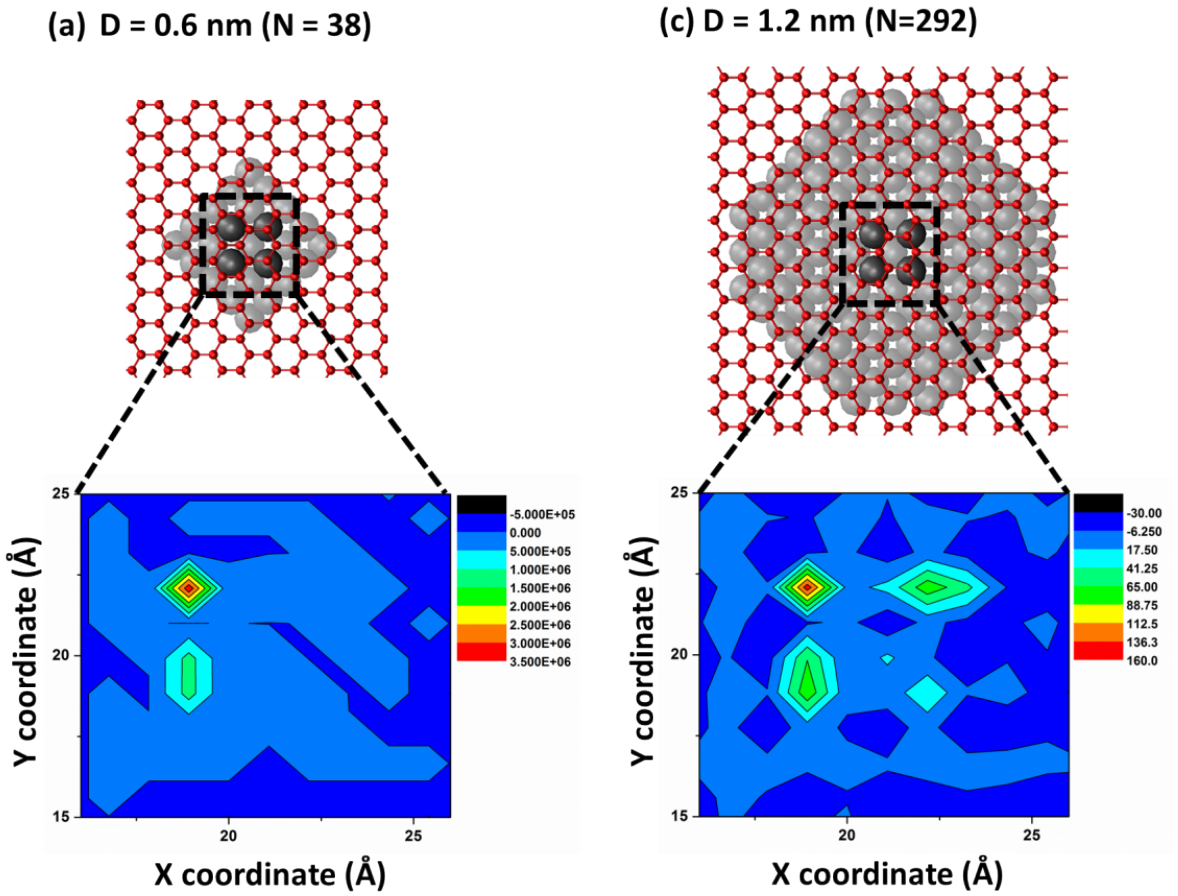

Figure S3. Potential energy surface for the different tip size. Graphene is represented by red sphere and silicon tip is represented by gray sphere. Darker sphere of silicon atoms represents the closest silicon atoms from graphene surface. Tip radiuses are (a) 0.6 nm and (b) 1.2 nm. Both cases have 4 closest atoms. PES shows the initial energy state of two tips. The case with the radius of 0.6 nm has two strong interaction points with the magnitude of interaction energy in order of 106. On the other hand, the case with the radius of 1.2 nm has four strong interaction points with the magnitude of interaction energy in order of 102.

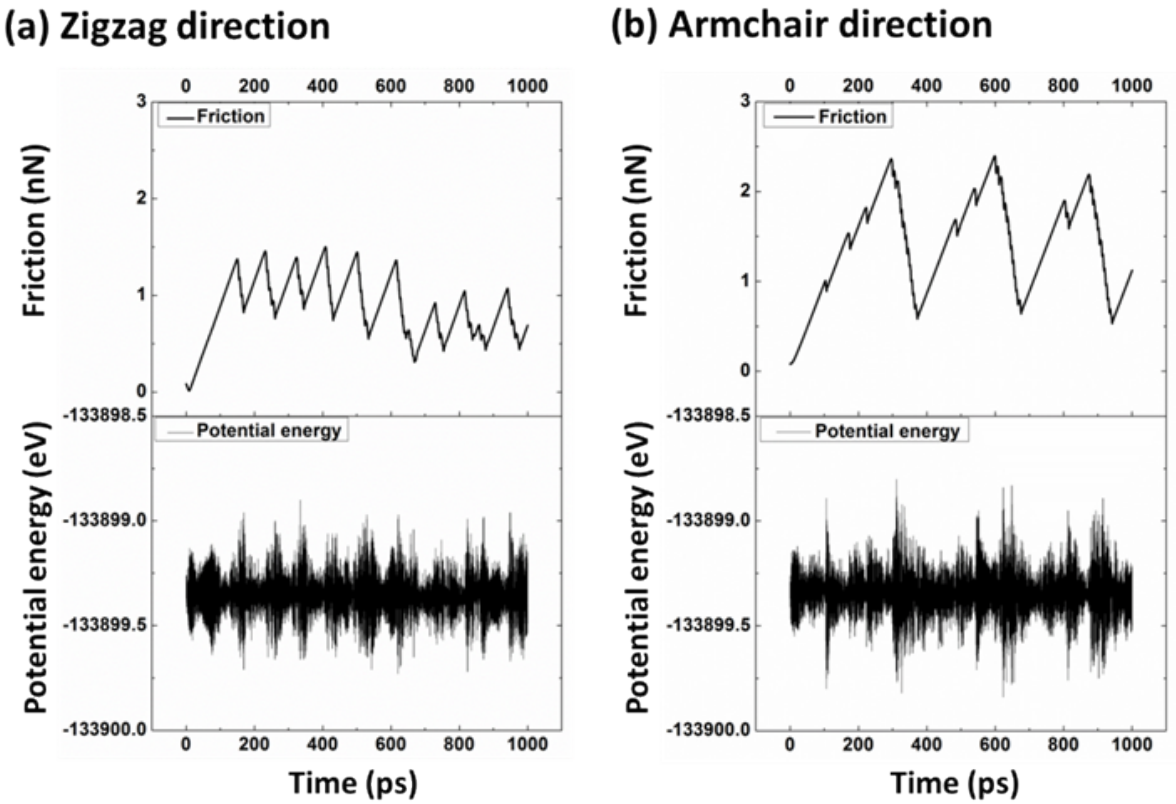

Figure S4. Variation of friction and potential energy for (a) zigzag and (b) armchair direction. Fluctuation in potential energy has drastically increased when slip event occurred. However, the potential energy fluctuated with the magnitude of 0.7 and 1.0 eV for zigzag and armchair direction, respectively.

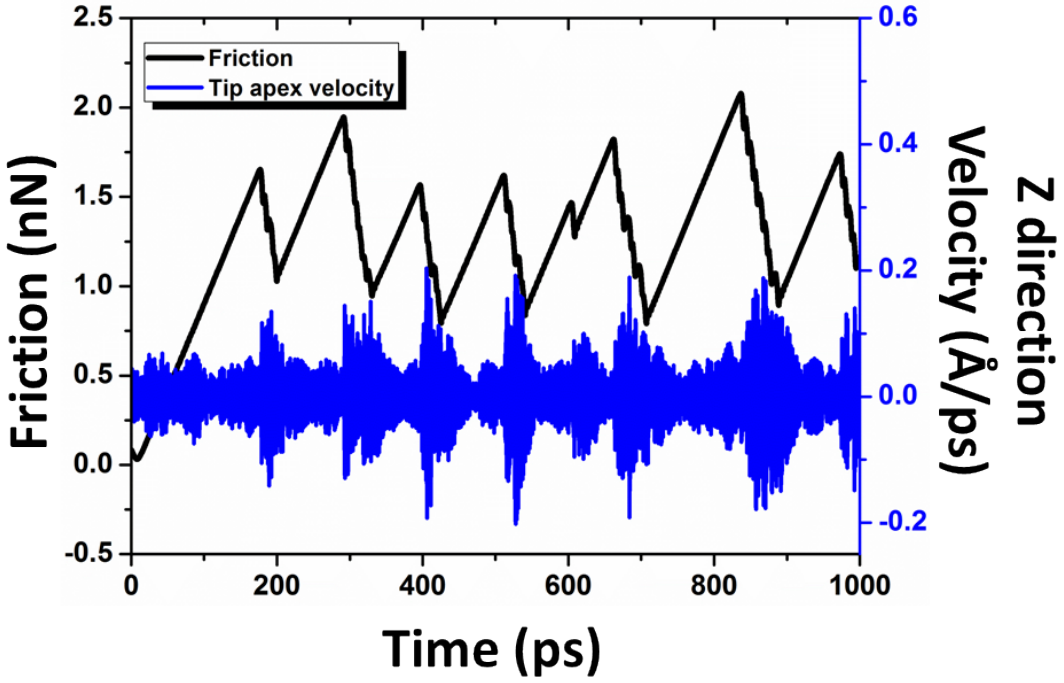

Figure S5. Friction vs. z-direction motion for type 1 simulation. The magnitude of fluctuation of the velocity increases when nanoscale slip motion occurs.

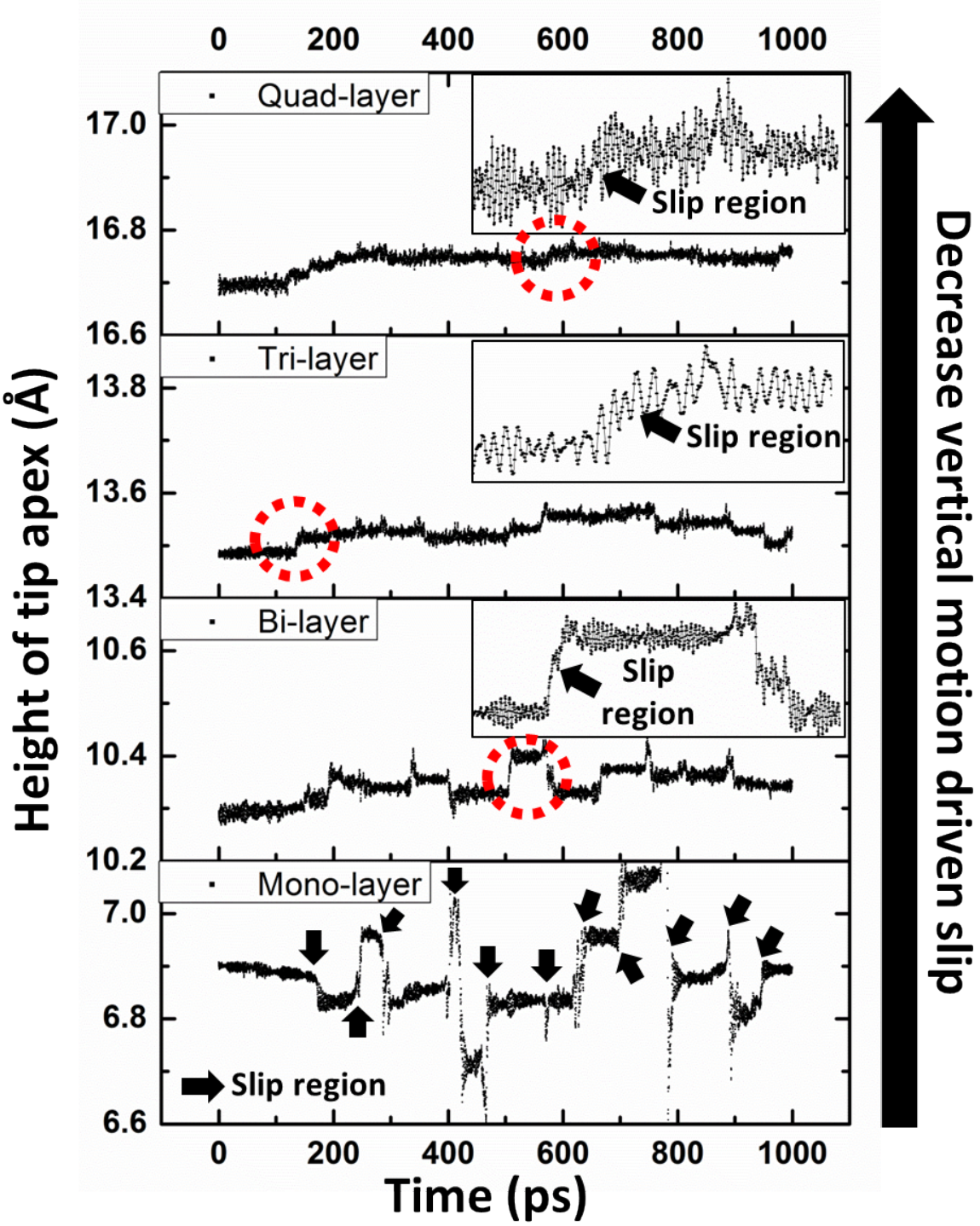

Figure S6. Effect of graphene thickness on vertical motion of the tip apex. An increase in the layer thickness decreases the effect of vertical motion.