(Supporting Information)

Atomistic mechanisms of superlubricity in carbon nanotube heterostructures under linear elastic deformation

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Supplementary Materials 1| The critical normal force required for the collapse deformation of nanotube is calculated, as shown in Fig. S1. The transition from linear elastic deformation to the collapsed states exhibits a nonlinear relationship between the force and tube size, as the critical force is proportional to the inverse cube of tube radius. This is in agreement with the previous results demonstrating that the structural transition of single-walled carbon nanotube (SWCNT) relating to hydrostatic pressure [1, 2].

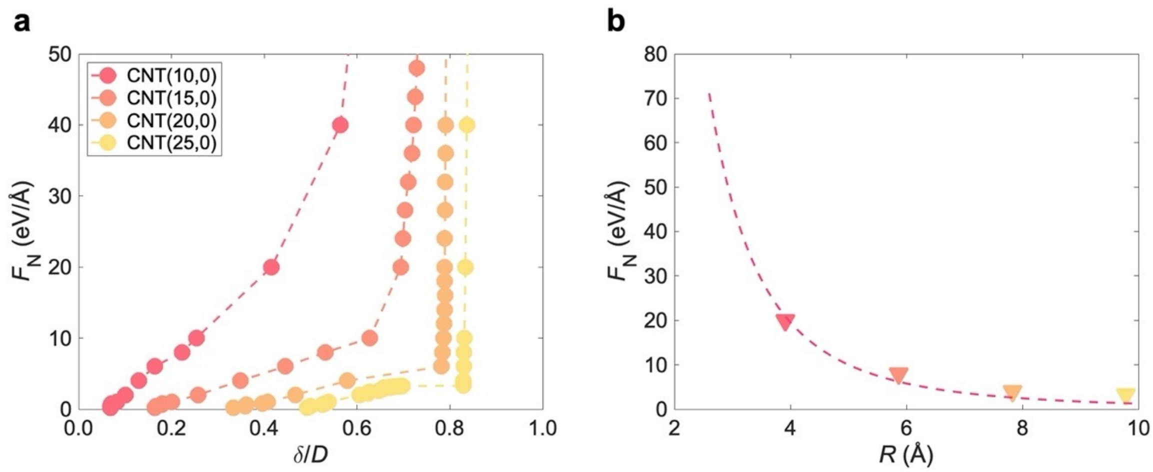

Fig. S1 Relationship between normal force and deformation of SWCNT.
(a) Normal force as a function of radial strain. (b) Critical force corresponding to the transition from linear elastic deformation to the collapsed state. The dashed line represents a cubic fit.

Supplementary Materials 2| The influence of thermal effects on nanotube motion induces diffusive behavior under small loads. As shown in Fig. S2, the rolling ratio and interfacial shear stress, both dependent on radial deformation at an ambient temperature of 300 K, are presented. The thermally induced diffusive motion of the nanotube causes fluctuations in rolling under small deformations. However, the rolling ratio in the linear elastic deformation regime fits well to a cubic equation, as shown in Fig. S2a. The critical deformation for the motion transition is similar to that observed at a lower temperature of 0.1 K. Moreover, temperature has minimal influence on the shear stress distribution, as shown in Fig. S2b.

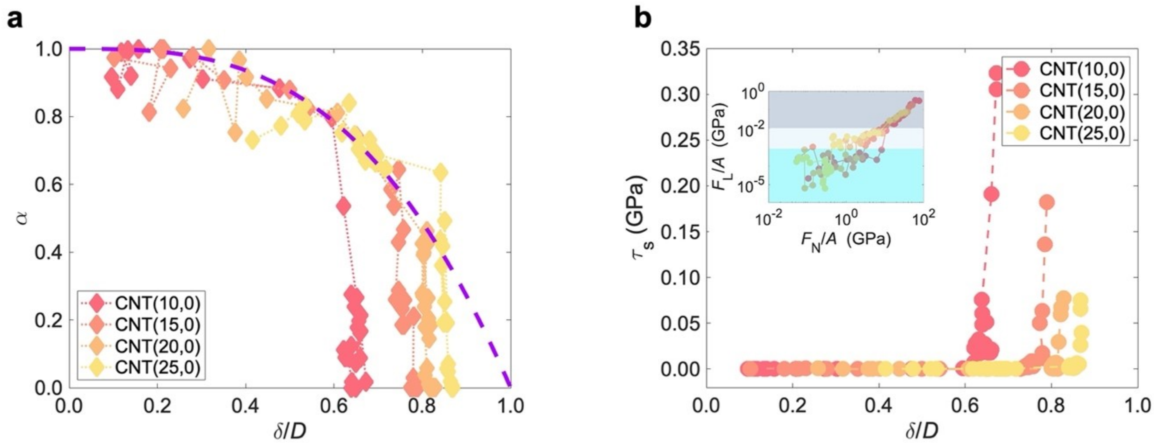

Fig. S2 Rolling ratio and interfacial shear stress as functions of deformation rate at ambient temperature (*T*=300 K).

(a) Rolling ratio (α) versus deformation rate (δ/D). The dashed violet line represents the theoretical model predicting the rolling ratio in the linear elastic deformation regime. The dashed line is plotted using the equation of $\alpha = 1 - \lambda^3$, where $\lambda = \delta/D$. (b) Shear stress (τ_s) as a function of deformation rate. The inset shows the distribution of area-normalized friction force versus normal force.

Reference

[1] Sun D Y, Shu D J, Ji M, Liu F, Wang M, Gong X G. Pressure-induced hard-to-soft transition of a single carbon nanotube. *Physical Review B* **70**(16): 165417 (2004)

[2] Hasegawa M, Nishidate K. Radial deformation and stability of single-wall carbon nanotubes under hydrostatic pressure. *Physical Review B* **74**(11): 115401 (2006)