SUPPLEMENTANTATY INFORMATION

# Two Distinct Buckling Modes in Carbon Nanotubes Bending


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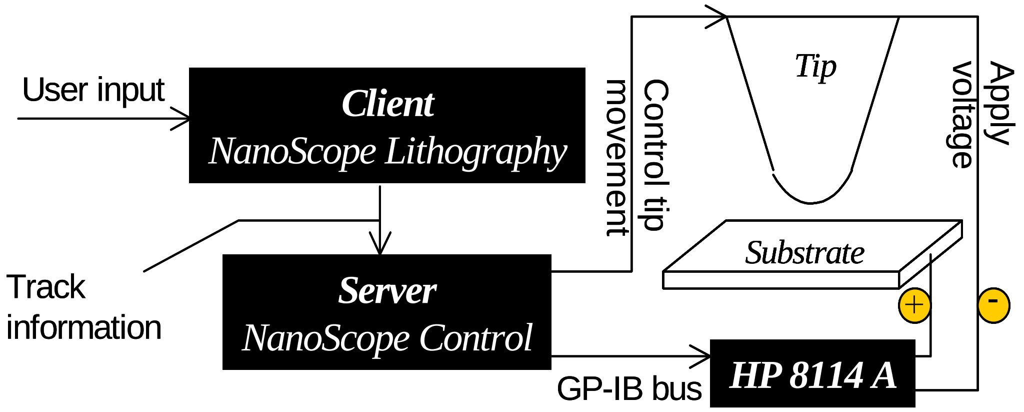
## Part I: Bending carbon nanotubes by SPM




**Scheme 1**. Schematic drawing of the SPM manipulation platform. The probe movements were controlled by homemade software designed using client-server architecture. The client program (Figure 1) displayed SPM images and provided methods to interact with operators to define manipulation tracks in a point-and-click style. Each track possessed parameters (e.g. feedback, setpoint, velocity) that could be easily set through dialog panels. The client program translated the information of tracks into coordinates and working parameters governing probe movements, which could be understood by the server program (Figure 2). Upon the receival of translated information, the server program started to move the probe and finish the manipulation. This platform can also be used to do the lithography. The function of the HP 8114A Programmable Pulse Generator is to apply voltages on samples when doing the nano-lithography .

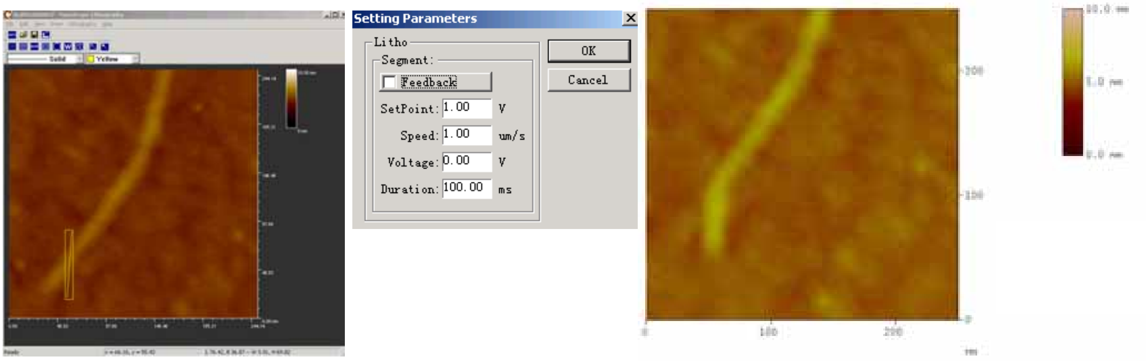



**Figure 1.** The interface of the client program. As shown in the left image, one track was defined to cross the carbon nanotube. For each track, the parameters were set in the dialog panel shown in the middle image. In this particular case, the tip would translate along the straight line with the feedback turned off at a speed of 1 µm/s (the server program intentionally disabled the interpretation of 1.0 V setpoint shown in the middle panel). The duration of 100 ms is meaningless for such a manipulation where the voltage was set as zero. The tip-sample distance was decreased by 10 nm as shown in Fig. 2 (depending on the original separation between tip and substrate, the decreased distance could be other values to establish an optimal contact load at the tip-substrate interface which is critical for the controlled bending); The right image shows the result of the manipulation under the conditions described above.

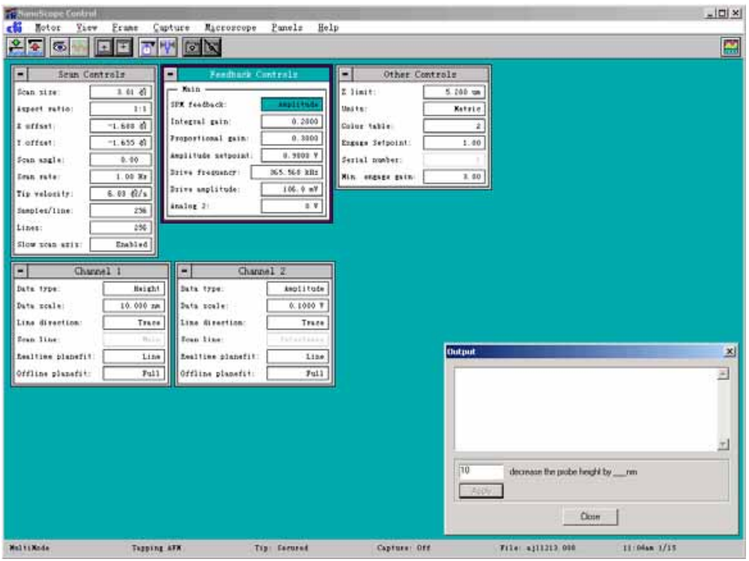
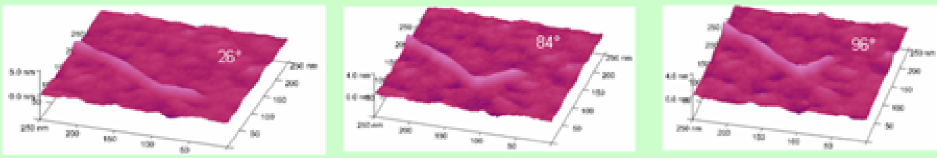


**Figure 2.** The server program shown in the lower-right corner of this figure was loaded from NanoScope Control as a dll (details could be found in the NanoScope Command Reference Manual). It opened a window to receive the broadcasted messages and used a file-mapping object to exchange data with the client program. The decrease of tip-sample distance was also set here.

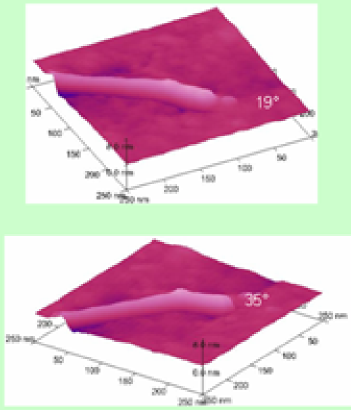
## Part II: Supplementary Data

(a)




(b)

| Bending angle (Degree) | H (nm) | ΔH (nm) |
|---|---|---|
| 0 | 3.17 | 0 |
| 3 | 3.53 | 0.05 |
| 19 | 3.43 | -0.05 |
| 35 | 4.50 | 1.02 |
| 44 | 4.61 | 1.13 |
| 48 | 4.67 | 1.19 |
| 53 | 4.45 | 0.97 |
| 64 | 4.54 | 1.06 |
| 77 | 4.61 | 1.13 |




(c)

| Bending angle (Degree) | H (nm) | ΔH (nm) |
|---|---|---|
| 0 | 2.82 | 0 |
| 38 | 3.03 | 0 |
| 50 | 3.04 | 0.01 |
| 53 | 3.17 | 0.14 |
| 57 | 3.29 | 0.26 |
| 63 | 3.24 | 0.21 |
| 78 | 3.30 | 0.27 |
| 91 | 3.45 | 0.42 |
| 110 | 3.44 | 0.41 |
| 120 | 3.42 | 0.39 |
| 130 | 3.41 | 0.38 |

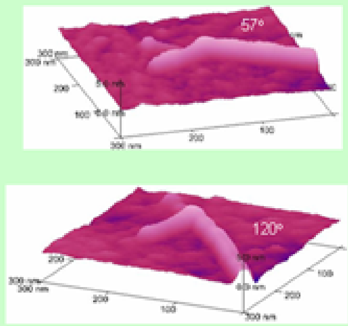



**Figure S1.** (a) 3-D AFM height images of the carbon nanotube with diameter of 1.31 nm bent to 26°, 84° and 96°. Tables in (b) and (c) show the heights and height changes (ΔH) at the bend "point" for tubes with 3.17 nm and 2.82 nm respectively. The calculation method is same with the carbon nanotube of 1.31 nm (details can be found in the manuscript). The right figures are the 3-D height images of the bent carbon nanotubes with different angles.

## Part III: Molecular dynamics study of vdW interaction effect on CNTs buckling

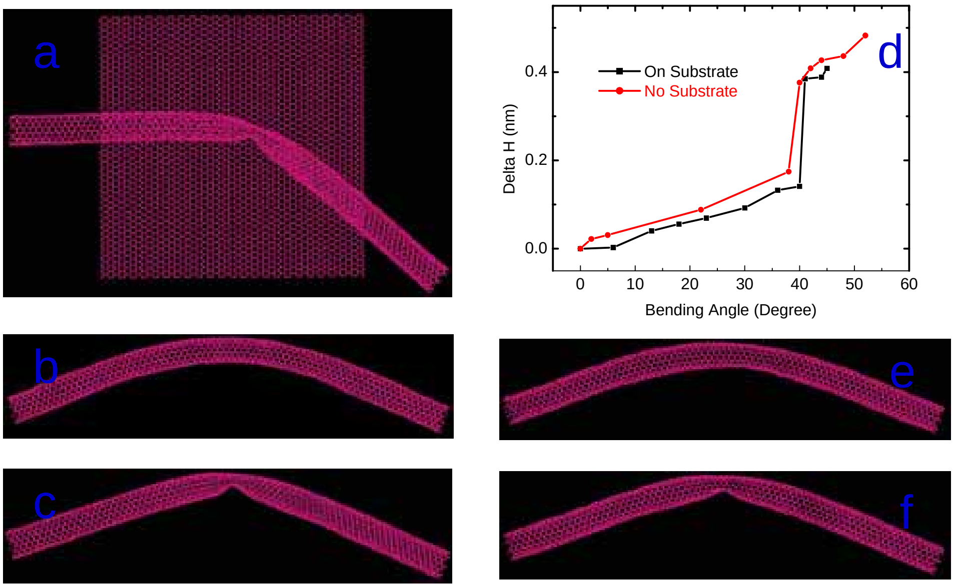



**Figure S2.** Molecular dynamics studies of influence of substrate on buckling of a (8,8) SWNT under bend loadings; (a) The overall configuration of a buckled (8,8) SWNT on a graphene substrate; (b) and (c) Side view of the geometrical configurations of the (8,8) SWNT before and after buckling which interacts with substrate by vdW force, for the convenience of comparison, the underlying graphene layer is not shown here; (d) Comparison of ΔH variation with respect to bending angle for SWNT with and without substrate; (e) and (f) Geometrical configurations of the isolated (8,8) SWNT before and after buckling.

As shown in Fig. S2, the simulation was conducted on an (8, 8) SWNT. To simply the simulation, a monolayer graphene rather than the silicon surface was used. These two surfaces should have no distinct difference in the vdW interaction. The distance between CNTs and surface has been set as 0.34 nm. The (8,8) SWNT has 2400 atoms and is 1.08 nm in diameter and 18.4 nm in length, the graphene layer has a size of $10.1\times9.9$ $nm^2$ and contains 4032 atoms. Limited by the calculation ability, the graphene layer is not large enough to cover the SWNT entirely, but because of the symmetry of the bend loading, the buckling position of the SWNT can be controlled to be located at the center of the graphene layer, therefore this would not influence the results of the vdW effect on the buckling behavior of the carbon nanotube (see Fig.S2a). For comparison, simulation of the (8,8) SWNT without substrate was also conducted, and the bend loadings were applied in the same scheme for both models as described in the text.

The variation of ΔH with respect to the bending angle is shown in Fig.S2d. From Fig.S2, it can be seen that the overall configuration, the critical buckling angle and the jump amplitude in ΔH at the critical buckling angle have no significant differences between the two cases with and without substrate, suggesting that when the SWNT is physically adsorbed on a substrate, the influence of the substrate on the buckling of carbon nanotubes can be neglected. This greatly simplified our system and made the experimental and theoretical results comparable.

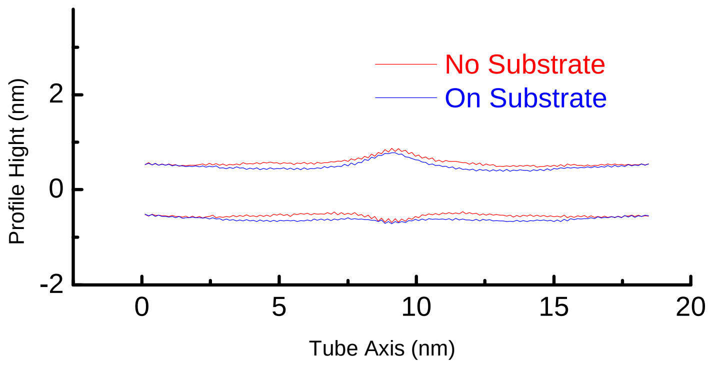



**Figure S3.** Contour plot of the buckled (8,8) SWNT profile under bend loadings.

Fig. S3 shows the contour plot of the buckled (8,8) SWNT profile under bend loadings. Except a little smooth of the lower side wall for tube on surface, no remarkable difference can be found between the two cases with and without surface.