

# Supporting Information

## **Mechanical properties of polygonal carbon nanotubes**

Ling Huang and Dapeng Cao\*

Division of Molecular and Materials Simulation, State Key Lab of Organic-Inorganic  
Composites, Beijing University of Chemical Technology, Beijing 100029, China

This supporting information provides (1) Comparison of number of atoms per unit cell and transverse size for P-/C-CNTs; (2) TST fitting for 3-,5-,6-,and 8-CNT.

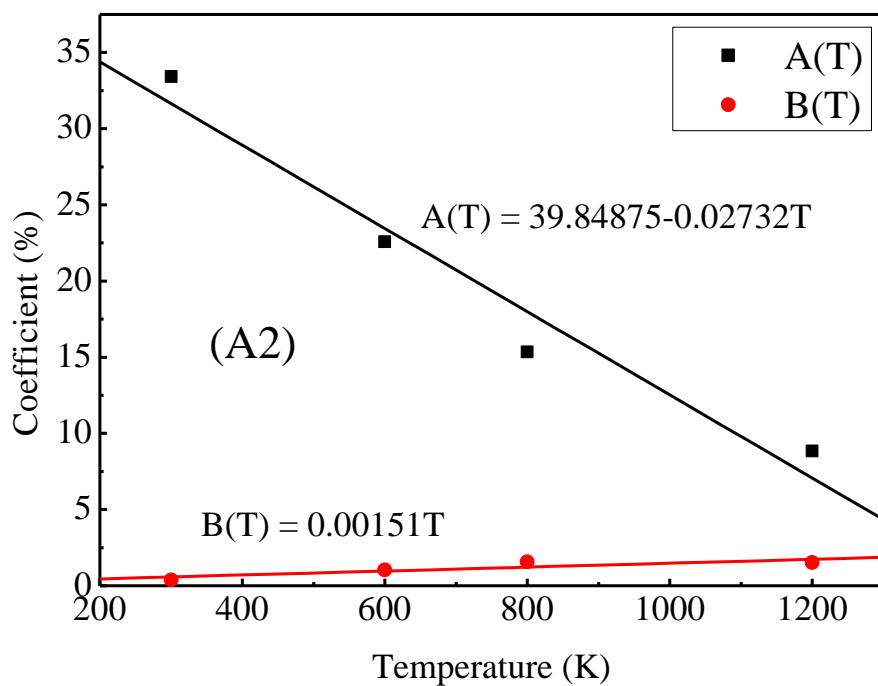
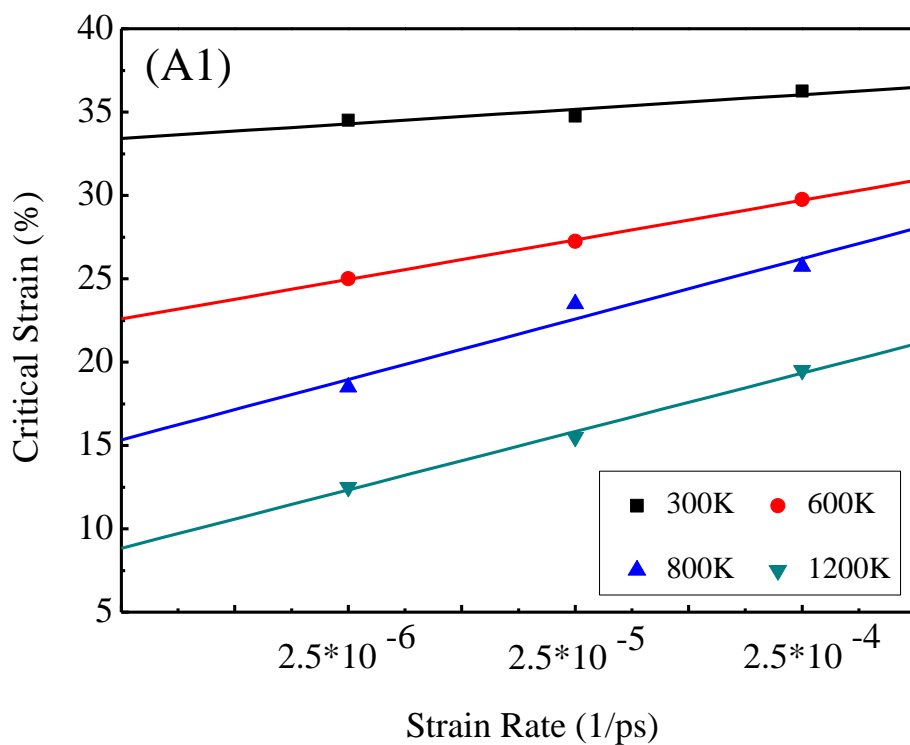
---

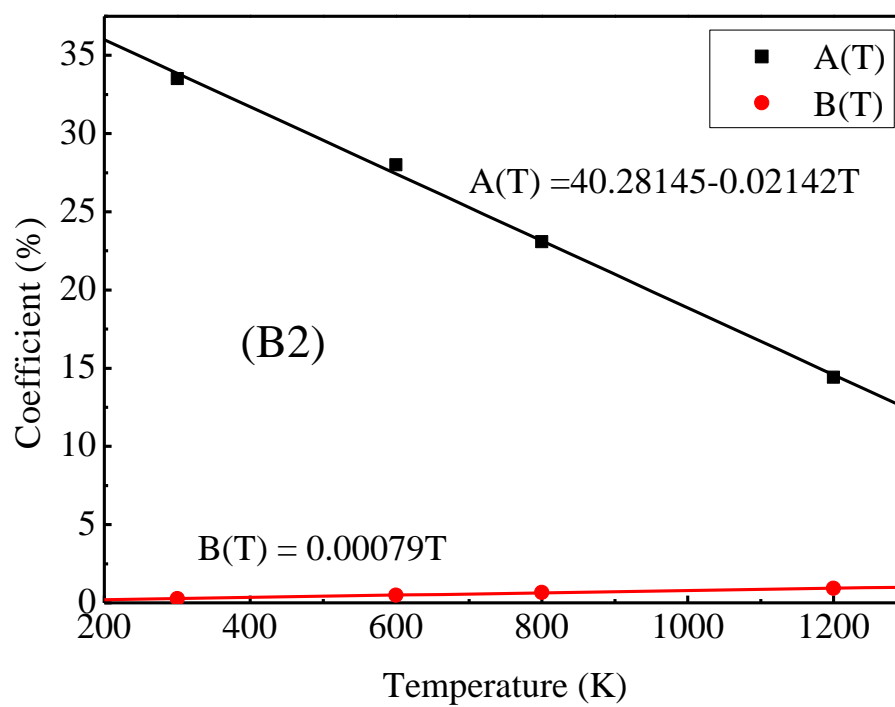
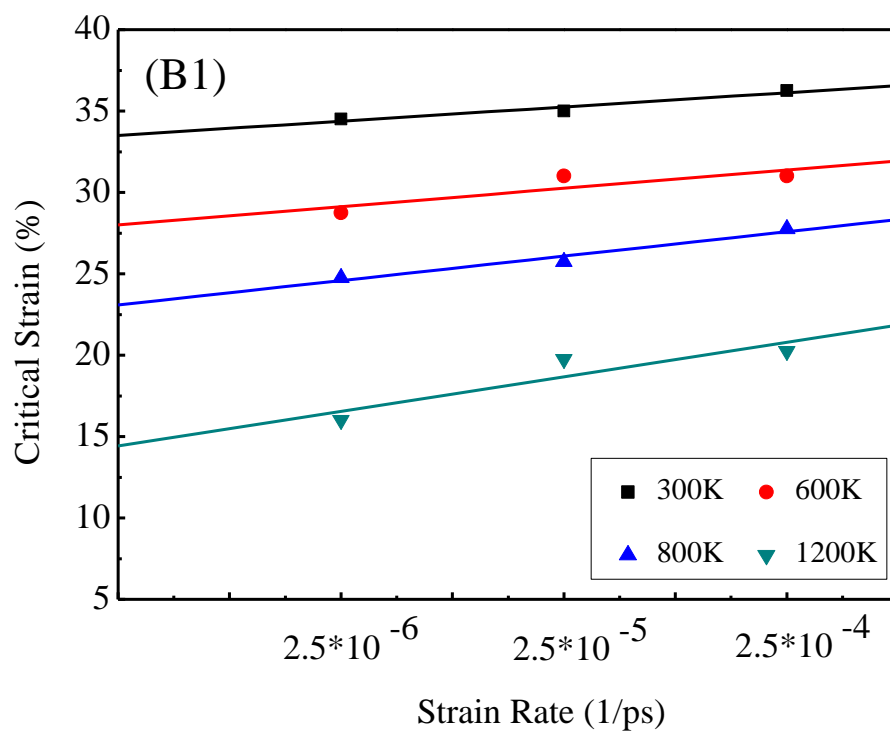
\*Corresponding author. Tel: +(86)10-64443254, Fax: +(86)10-64427616 E-mail address:  
[caodp@mail.buct.edu.cn](mailto:caodp@mail.buct.edu.cn) (D.P. Cao)

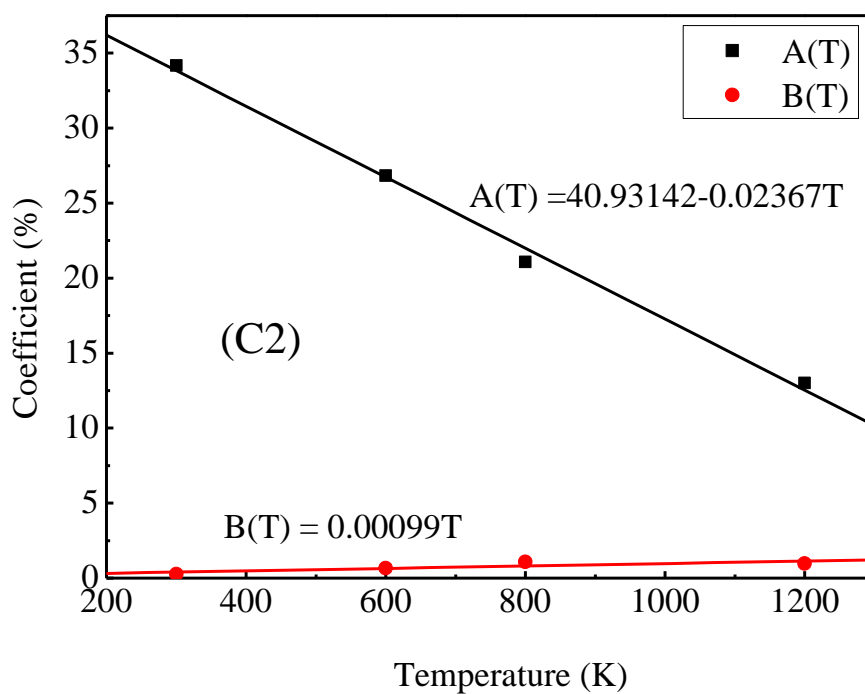
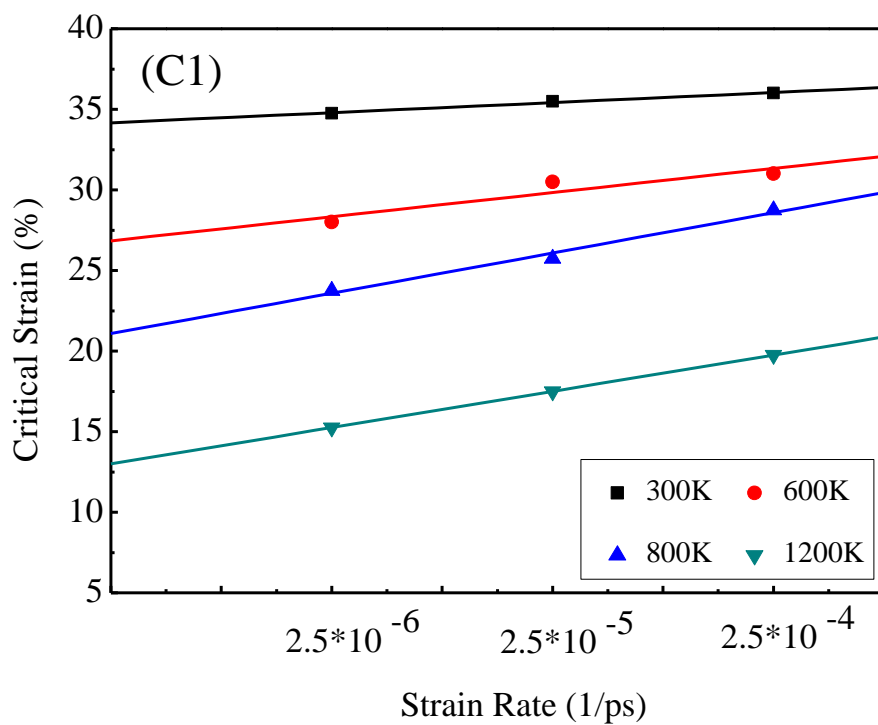
**Table S1.** Comparison of number of atoms per unit cell and transverse size for P-CNTs and C-CNTs. The formulas for transverse size was presented in Figure 2.

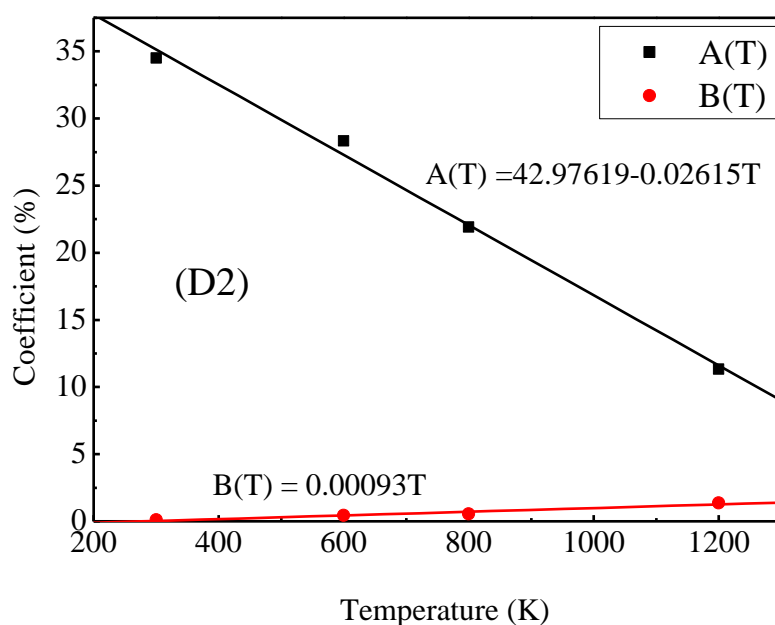
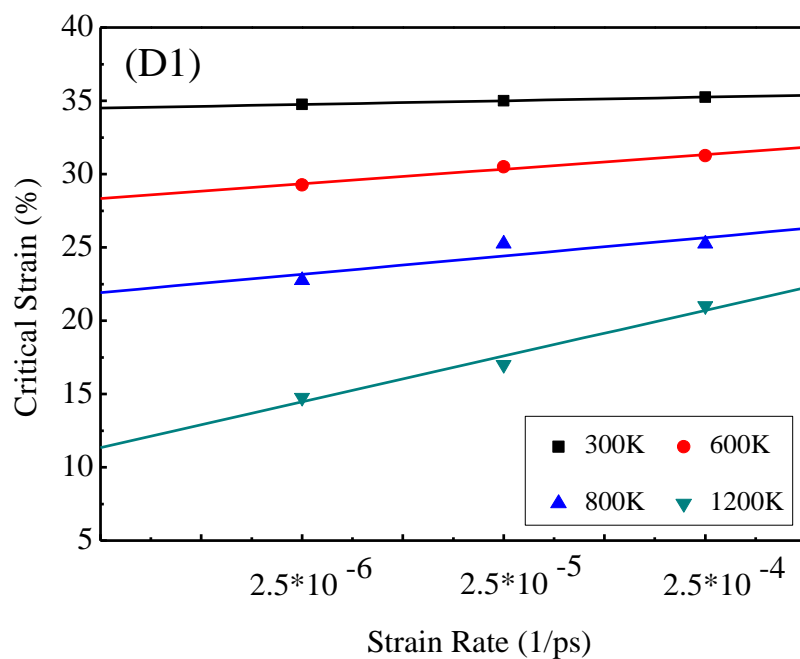
| Number of atoms per unit cell      |         |        |         |         |         |
|------------------------------------|---------|--------|---------|---------|---------|
| P-CNTs                             | 3-      | 4-     | 5-      | 6-      | 8-      |
|                                    | 15      | 20     | 25      | 30      | 40      |
| C-CNTs                             | (5,5)   | (6,6)  | (7,7)   | (8,8)   | (11,11) |
|                                    | 20      | 24     | 28      | 32      | 44      |
| Transverse size ( $\text{\AA}^2$ ) |         |        |         |         |         |
| P-CNTs                             | 3-      | 4-     | 5-      | 6-      | 8-      |
|                                    | 127.923 | 124.44 | 141.784 | 159.793 | 197.154 |
| C-CNTs                             | (5,5)   | (6,6)  | (7,7)   | (8,8)   | (11,11) |
|                                    | 72.383  | 86.903 | 101.315 | 115.835 | 159.286 |

### TST fitting for 3-,5-,6-,8-CNTs.









**Figure S1.** (A1), (B1), (C1), and (D1) represent critical strain of P-CNTs (3-CNT, 5-CNT, 6-CNT, and 8-CNT, respectively) as a function of the strain rate at different temperatures. (A2), (B2), (C2), and (D2) represent the fitting of A(T) and B(T) for 3-CNT, 5-CNT, 6-CNT, and 8-CNT, respectively, where A(T) and B(T) are denoted as functions of temperature.