ANOMALOUS RESISTANCE CHANGE OF ULTRASTRAINED INDIVIDUAL MWCNT USING MEMS-BASED STRAIN ENGINEERING

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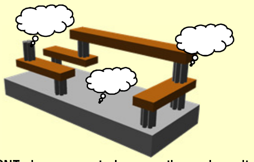
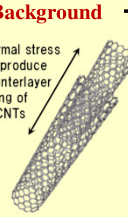
ABSTRACT : This research clarified the anomalous electric resistance change of ultrastrained multi-walled carbon nanotube (MWCNT), as well as its mechanical properties, using the Electrostatically Actuated NAnotensile Testing device (EANAT) mounted on the in-situ SEM nanomanipulation system. The Young's modulus of MWCNT and its shear stress during interlayer sliding deformation were estimated from the load-displacement curve. The electrical resistance of the MWCNT was 215 kΩ without strain, which was similar to the previously reported value, however the anomalous resistance change was observed under enormous strain. Although the resistance change ratio was almost constant during interlayer sliding of the MWCNT, it specifically showed a sharp raise at the end of the sliding in spite of the MWCNT not breaking mechanically. The molecular dynamics (MD) simulation provided a good understanding that the atomic reconfiguration due to the hard sticking at the edge of extracted outer layer of MWCNT might induce the sharp raise of resistance without its mechanically breaking. This result reported here is extremely important for reliability of MWCNT interconnects.

Background and Design of Device

Background





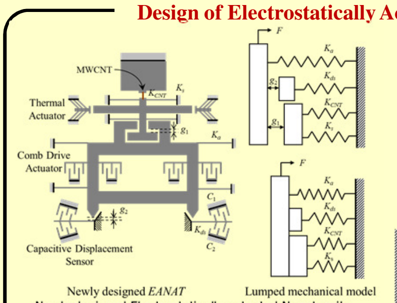
Thermal stress can produce the interlayer sliding of MWCNTs

MWCNTs have come to be recently used as ultra low resistances interconnect materials for via structures in micro devices

● Via structures formed by MWCNTs have to sustain thermal stress generated in the operation of micro devices, which can lead to the interlayer sliding deformation of MWCNTs resulted in changing electrical resistance. For a reliable design of MWCNTs interconnect, we need basic information of mechanical and electrical characteristics of individual MWCNTs.

● This research focuses on clarifying the stress-strain relation and the resistance change of individual MWCNT under its interlayer sliding deformation. The relationship between the resistance change and breaking mechanism of MWCNT are also examined by MD simulation.

Design of Electrostatically Actuate Nanotensile Testing Device



Newly designed Electrostatically actuated Nanotensile Testing Device (EANAT)

$$C_1 = C_0 + \Delta C_1 = C_0 + \Delta C_{side}^{dec} + \Delta C_{tip}^{dec}$$

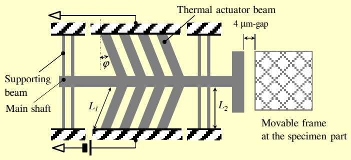
$$C_2 = C_0 + \Delta C_2 = C_0 + \Delta C_{side}^{inc} + \Delta C_{tip}^{inc}$$

$$C_0 = \sum_{k=1}^{n}\left\{\frac{\varepsilon_0 h\left(r_k^{ins} + r_k^{outs}\right)(\beta_0 - \alpha_0)}{d} + 2\cdot\frac{\varepsilon_0 h d}{D_k}\right\}$$

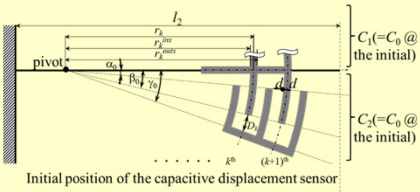
$$\Delta C_{side}^{dec} = -\Delta C_{side}^{inc} = \sum_{k=1}^{n}\left\{\frac{-\varepsilon_0 h \delta_k^{ins}}{d} + \frac{-\varepsilon_0 h \delta_k^{outs}}{d}\right\}$$

$$\Delta C_{tip}^{dec} = 2\sum_{k=1}^{n}\varepsilon_0 h d\left(\frac{1}{D_k + r_k\theta} - \frac{1}{D_k}\right)$$

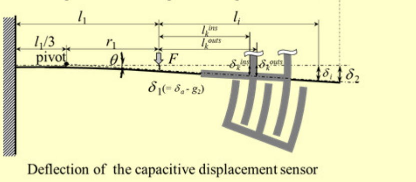
$$\Delta C_{tip}^{inc} = 2\sum_{k=1}^{n}\varepsilon_0 h d\left(\frac{1}{D_k - r_k\theta} - \frac{1}{D_k}\right)$$



Thermally driving actuator employed as a stopper



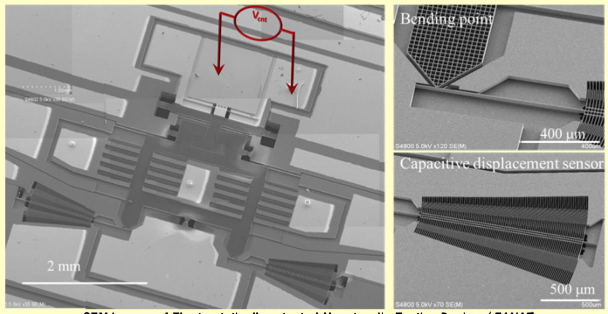
Initial position of the capacitive displacement sensor



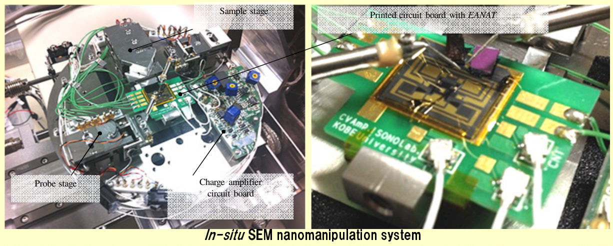
Deflection of the capacitive displacement sensor

Capacitive displacement sensor incorporated to cantilever motion amplification system

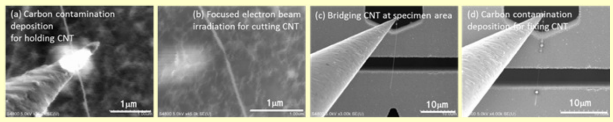
Experimental Tools for Strain Engineering of Nanowire



SEM images of Electrostatically actuated Nanotensile Testing Device (*EANAT*)



In-situ SEM nanomanipulation system

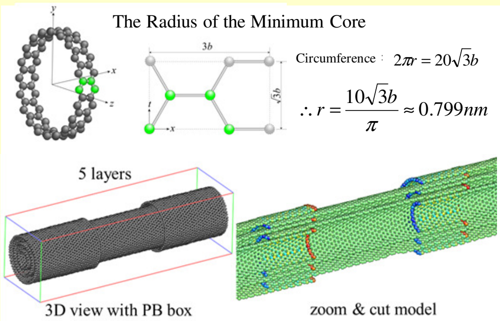


SEM images of nanomanipulating and fixing an individual MWCNT: (a) scooping up the MWCNT with the probe, (b) cutting the MWCNT by irradiation of focused electron beam, (c) approach of the probe with MWCNT to the specimen part, and (d) fixing the MWCNT on the device by the electron beam induced contamination.

●Each functional element was successfully fabricated on the device according to the design. The output signals from the charge amplifier were recorded in the memory storage with the 14 bit-AD convertor per ±5V at a period of 10 msec. The measurement resolution of displacement resulted in 0.28 nm in this case.

Results and Discussions

MWCNT Models for Molecular Dynamics Simulations



Five cylindrical shells

MD simulation models of MWCNTs with two, three and five cylindrical shells

$$E = \sum_i \sum_{j>i}\left[V_R(r_{ij}) - \overline{B_{ij}} V_A(r_{ij})\right]$$

$$V_R(r_{ij}) = f_c(r_{ij})\frac{D_{ij}^{(e)}}{S_{ij} - 1} exp\left(\sqrt{2S_{ij}}\beta_{ij}\left(R_{ij}^{(e)} - r\right)\right)$$

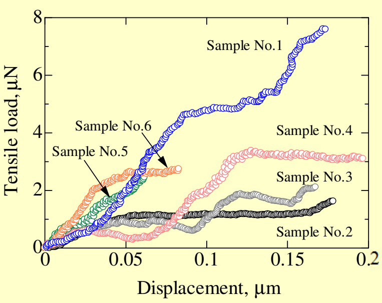
$$V_A(r_{ij}) = f_c(r_{ij})\frac{S_{ij}D_{ij}^{(e)}}{S_{ij} - 1} exp\left(\sqrt{\frac{2}{S_{ij}}}\beta_{ij}\left(R_{ij}^{(e)} - r\right)\right)$$

Bond-order empirical potential function proposed by D.W. Brenner

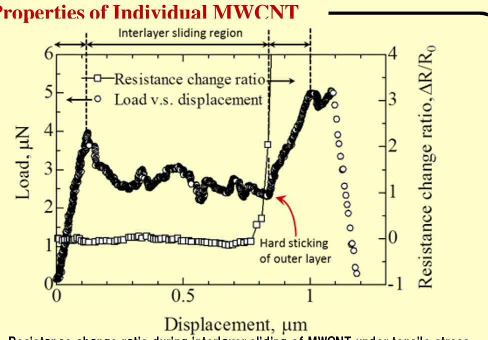
●We carried out classical MD simulations using the bond-order empirical potential function proposed by D.W. Brenner.

●The unit ring of carbon cylinder model with the minimum diameter of 1.59 nm is also shown in the figure, which is composed of zigzag structures in the longitudinal direction. The single CNT shell corresponds to 30 unit rings, and its length is 13.05 nm (=*L*). Thus, the total length of the telescopic MWCNT models is 19.6 nm (=1.5*L*) since the overlap region between the outer and inner shells is defined as 0.25L.

Mechano-Electrical Coupled Properties of Individual MWCNT



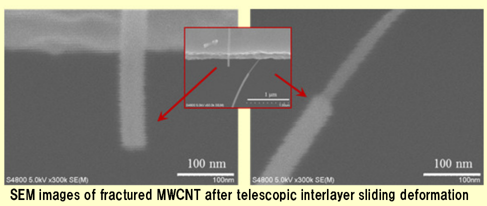
Load-displacement curves



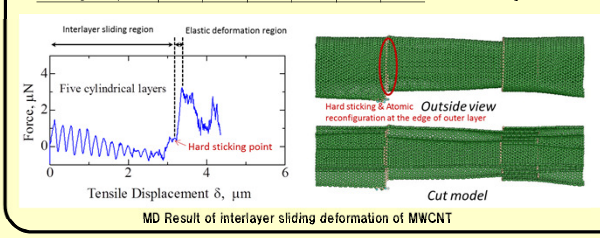
Resistance change ratio during interlayer sliding of MWCNT under tensile stress

Mechanical properties of MWCNTs synthesized by APCVD

Sample	No. 1	No. 2	No. 3	No. 4	No. 5	No. 6
Length (µm)	17.1	5.52	5.10	7.09	5.91	4.64
Diameter (nm)	51.5	30.0	31.3	35.9	32.3	33.5
Young's Modulus (GPa)						
the 1st increment	625	594	362	384	518	461
the 2nd increment	628	517	386	516	440	–
the 3rd increment	—	—	403	—	464	–
Tensile Strength (GPa)	3.72	2.35	2.78	2.81	3.56	3.33
Fracture Strain (%)	1.02	1.36	3.29	2.80	1.05	1.78
Elongation (µm)	0.174	0.179	0.168	0.198	0.062	0.083



SEM images of fractured MWCNT after telescopic interlayer sliding deformation



MD Result of interlayer sliding deformation of MWCNT

●The Young's modulus and the shear stress during the interlayer sliding showed 418 GPa, and 60.1 MPa, respectively. The electrical resistance of the MWCNT was 215 kΩ without strain. However, the anomalous resistance change was observed under enormous strain in the figure in spite of the MWCNT not breaking mechanically. The resistance change ratio was almost constant during the interlayer sliding, but it showed a sharp raise at the end of the sliding without breaking.

●The MD result suggested that the anomalous resistance change of MWCNT without mechanically breaking in the experiment was caused by the atomic reconfiguration due to hard sticking at the edge of the outer layer.

MEMS 2015 • 18-22 January, 2015 • Estoril, Portugal
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