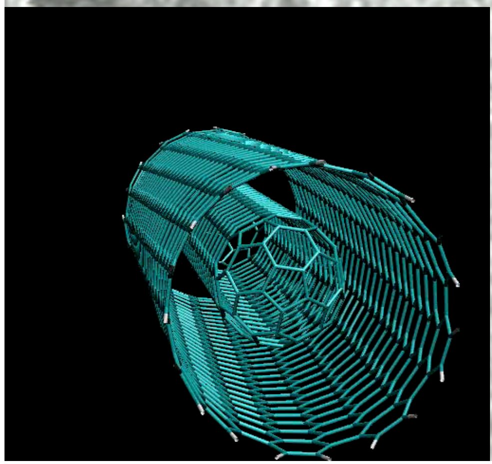
4th Int. Workshop on “Quantum Particles and Fields”
Sept. 19-24, 2005 Baku Azerbaijian

Metastable Deformation of Carbon Nanotubes

Y.Nakayama
Osaka Prefecture University
Osaka University



Outline

◎ What is a carbon nanotube (CNT) ?

◎ Manipulation of CNT in Nanofactory

(SEM with manipulator)

◎ Plastic deformation of CNT

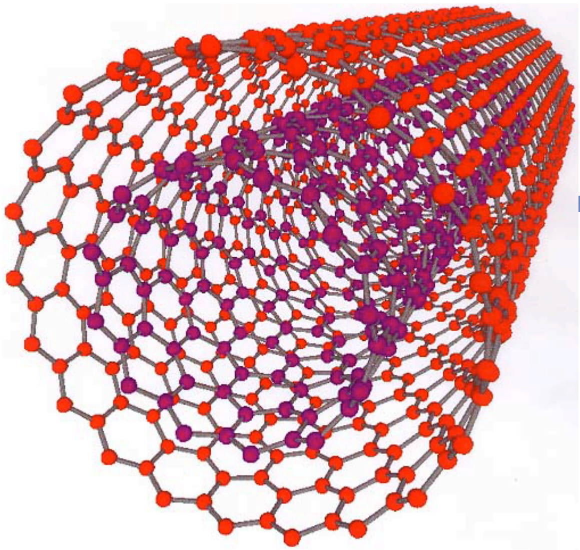
・Manipluration in Supernanofactory (TEM with manipulator)

◎ Recovery from the plastic-deformation

◎ Computer simulation

・Potential barriers for the plastic-deformation

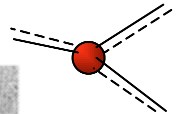
◎ Conclusion

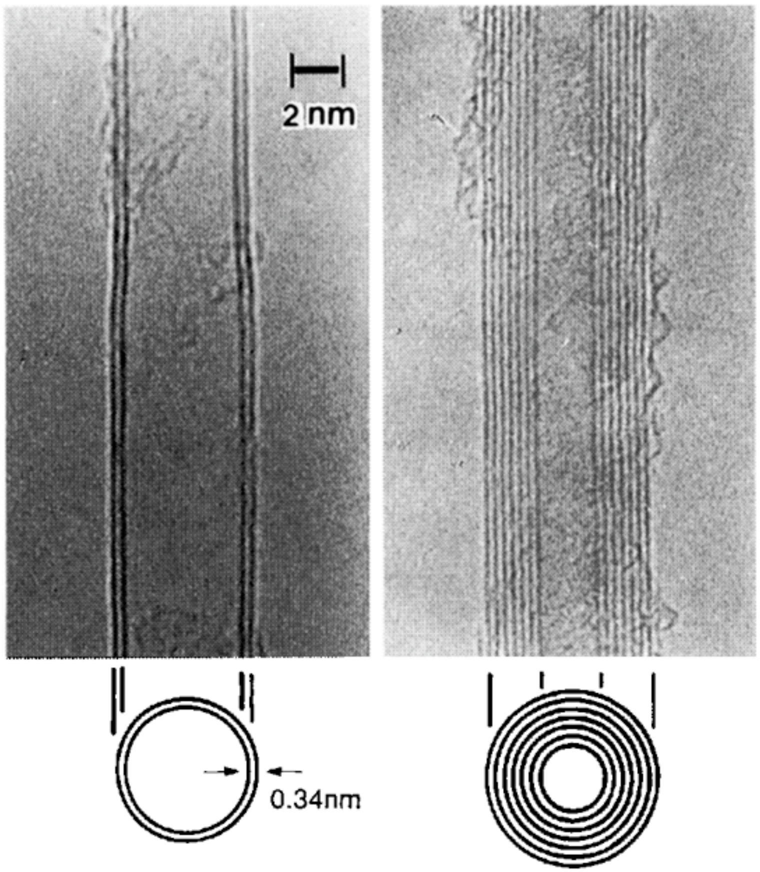


Discovery of Carbon Nanotube

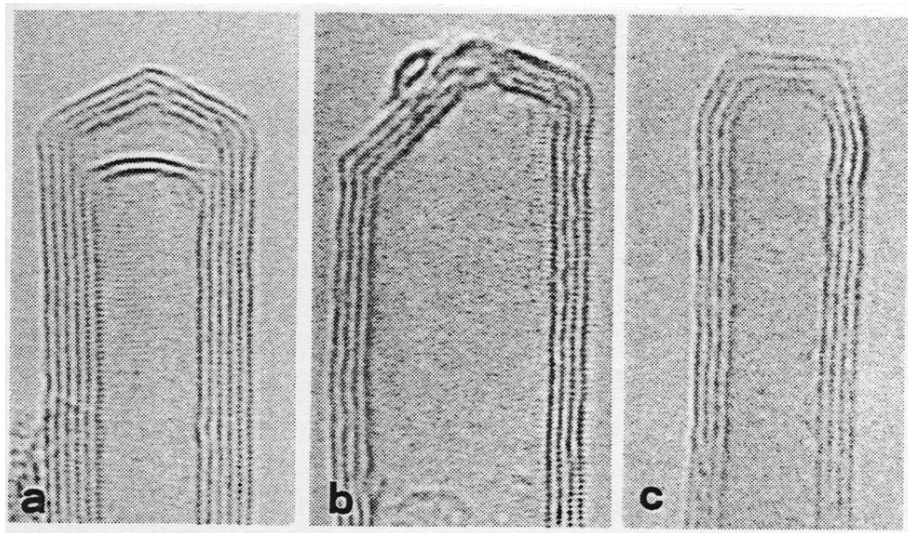
In 1991

sp^2 bonding

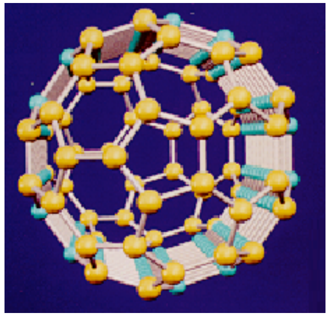
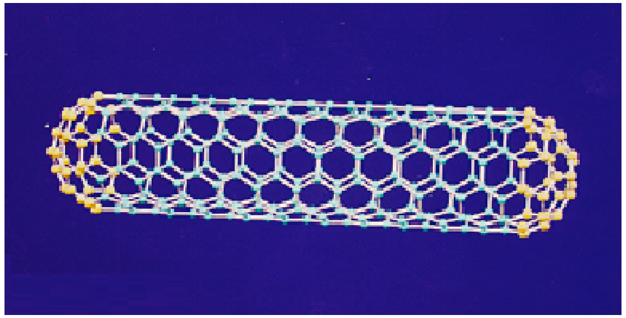




S Iijima, *Nature (London)* **354**, 56, (1991).

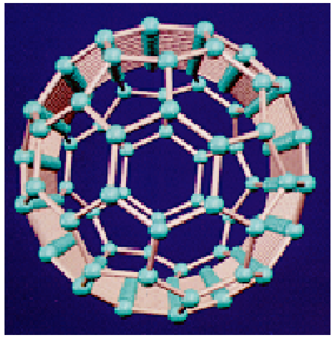
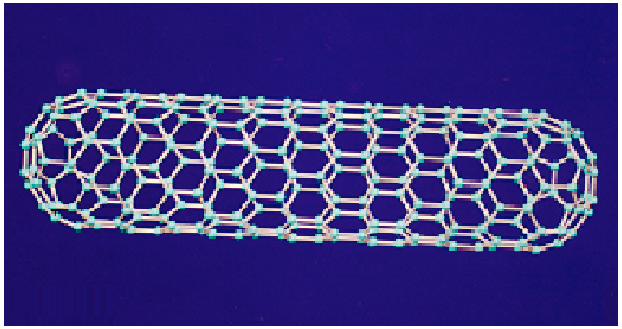


Carbon nanotubes

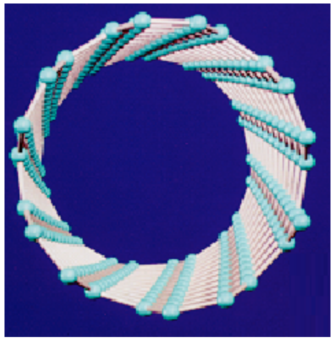
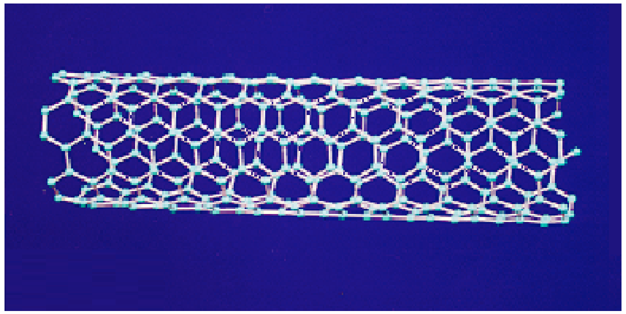
(5,5) Metal

Armchair nanotube

(9,0) Metal

Zigzag nanotube

(6,5) Semicond.

Chiral nanotube

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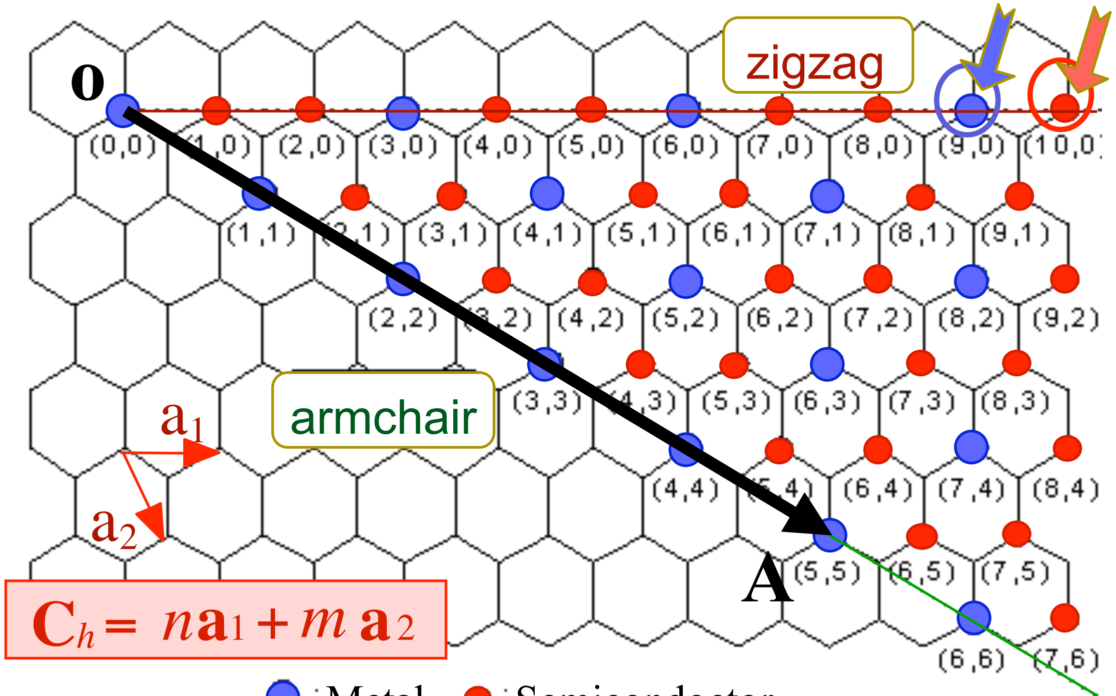
Energy Band

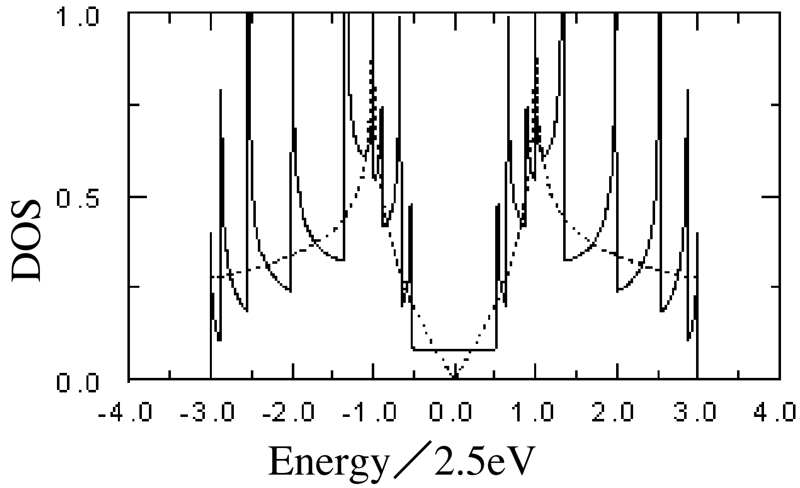
R. Saito *et al.,* Appl. Phys. Lett. **60**, 2204 (1992)



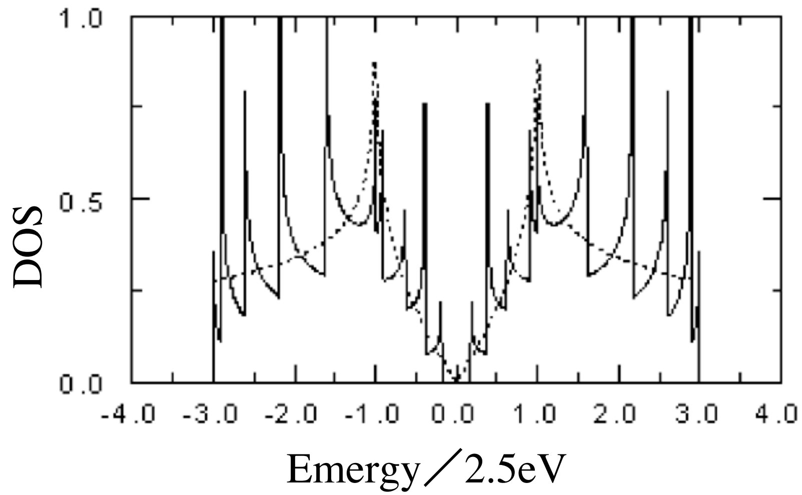
$C_h = n\mathbf{a}_1 + m\,\mathbf{a}_2$

● : Metal ● : Semicondoctor

(a) (n,m)=(9,0)



(b) (n,m)=(10,0)



$n - m = 3\ell$	⇨	Metal	1/3
$n - m \neq 3\ell$	⇨	Semicond.	2/3

Tough Nanotubes

http://www.lippmannforcongress.us/space.htm

sp^2 bond + (seamless structure)

Material	Young Modulous (GPa)	Strength (GPa)	Density (g/cm^3)
SWNT	1054	150	1.2
MWNT	1300	150	2.6
Steel	208	0.4	7.8

Applied Nanotechnology Inc. and Others

5 times tough and 1/5 density
as compared with steel

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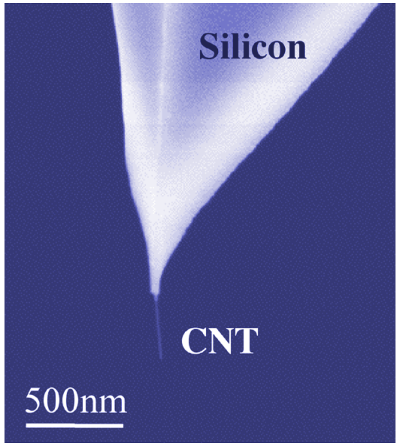
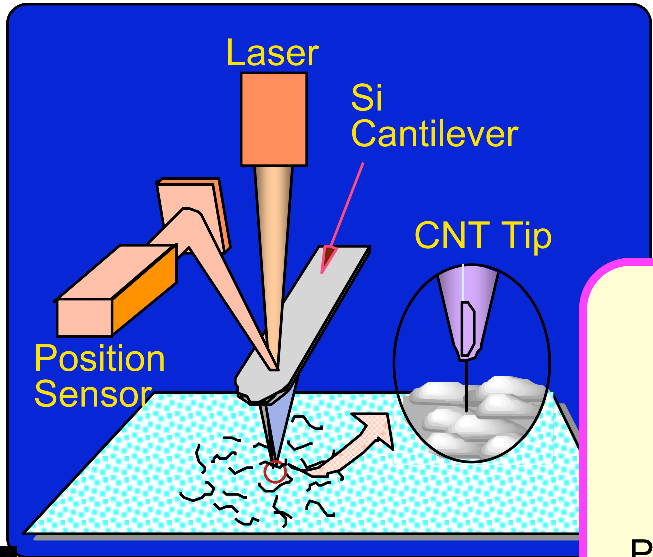
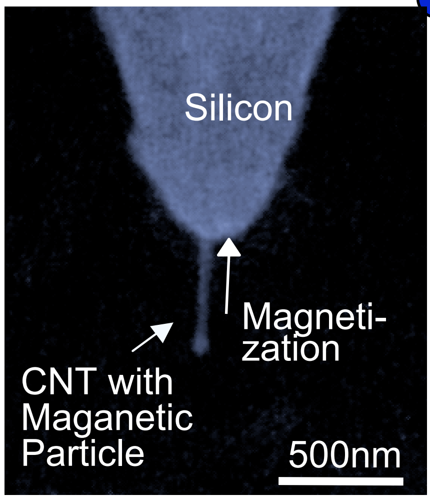
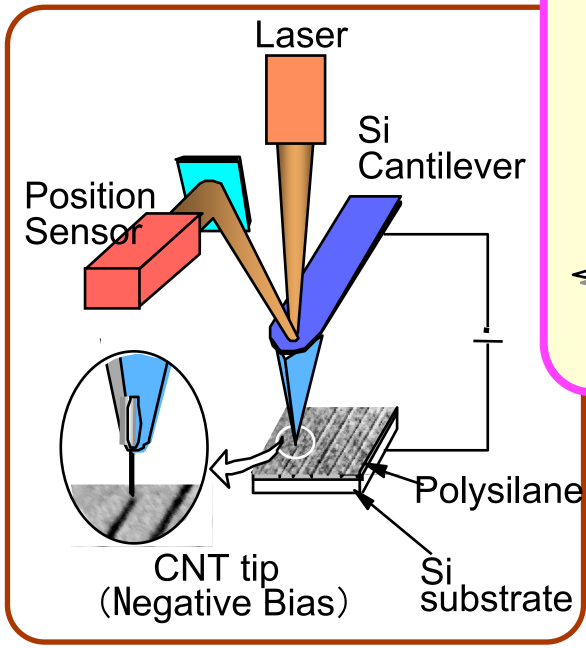
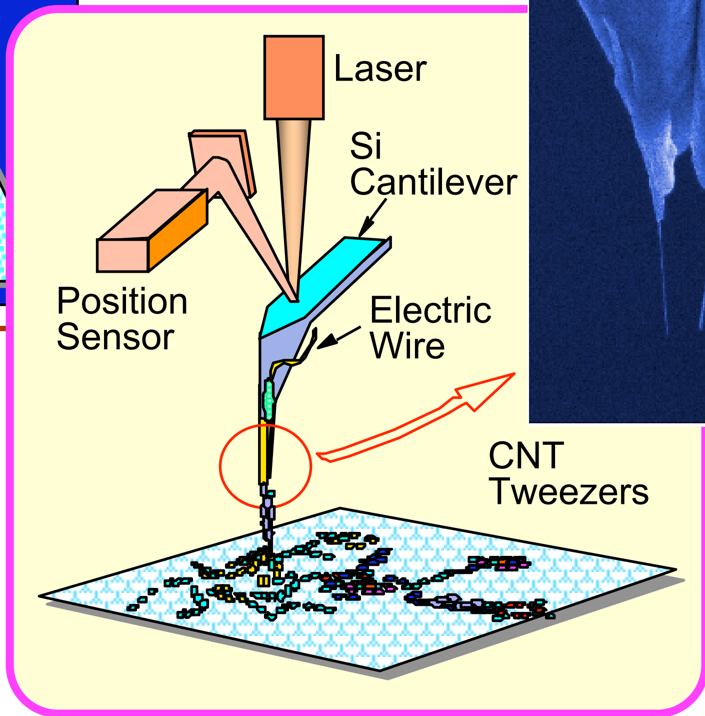
CNT tips and CNT tweezers

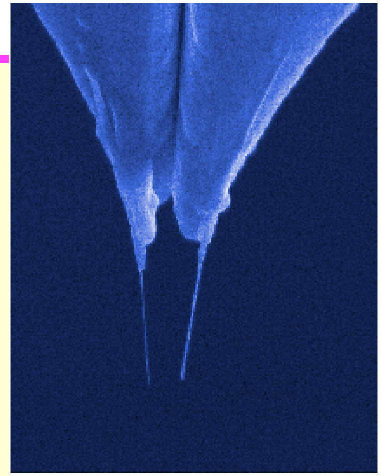












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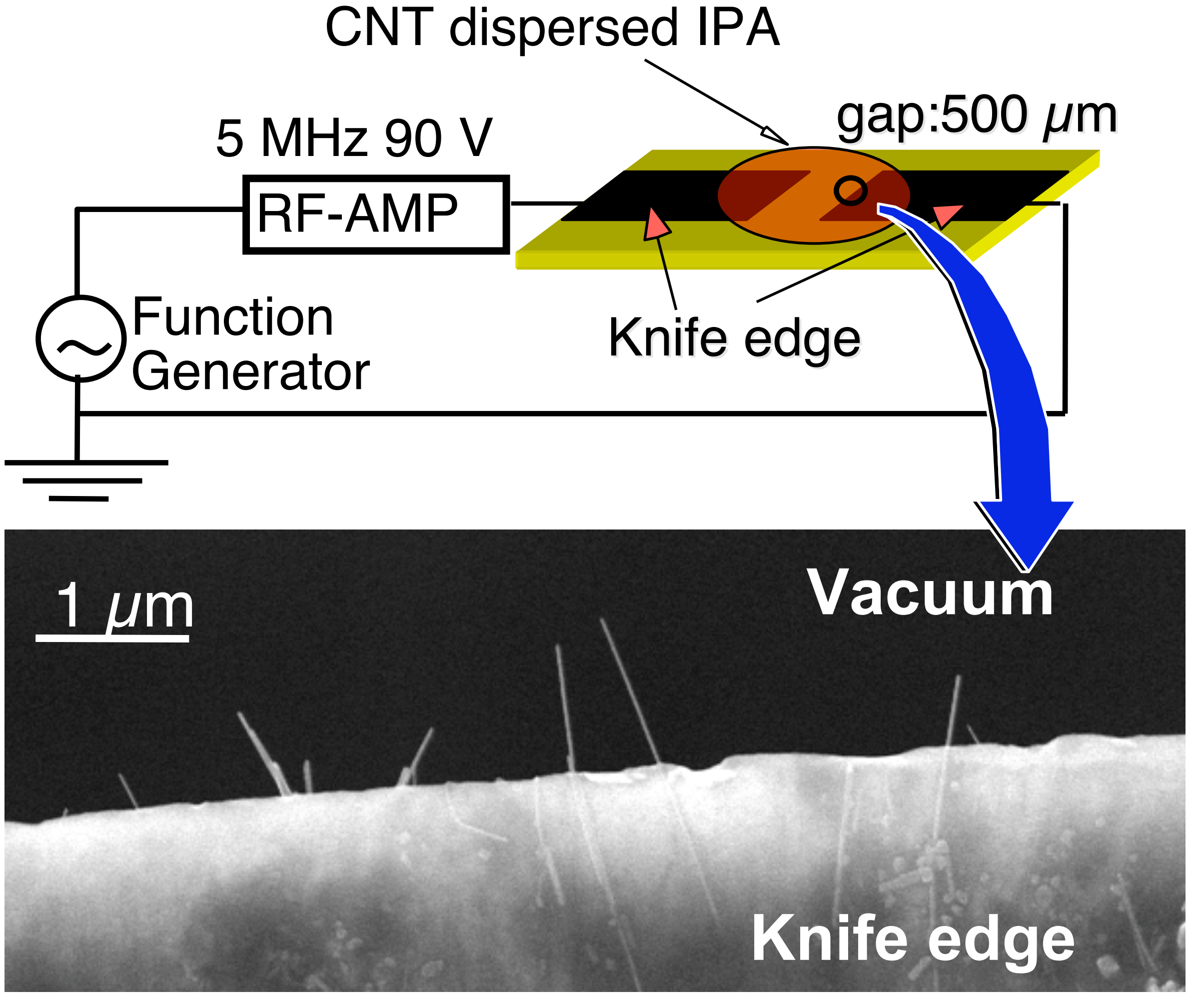
Preparation of CNT cartridge



CNTs are
- purified from the particles
- aligned on the knife edge

by ***dielectrophoresis***.

CNTs are protruded from the edge

Easy to handle!

K. Yamamoto et al, J. Phys. D **31**, L34 (1998).

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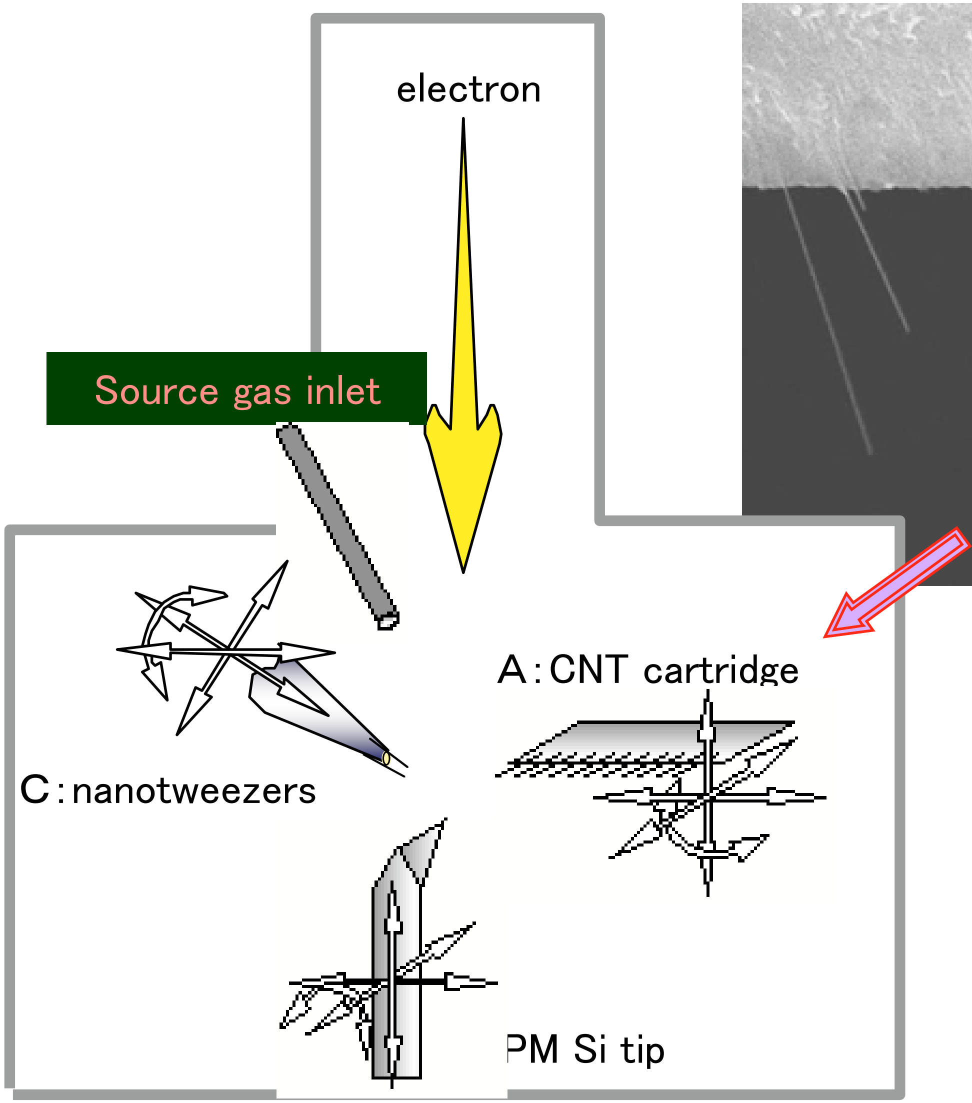
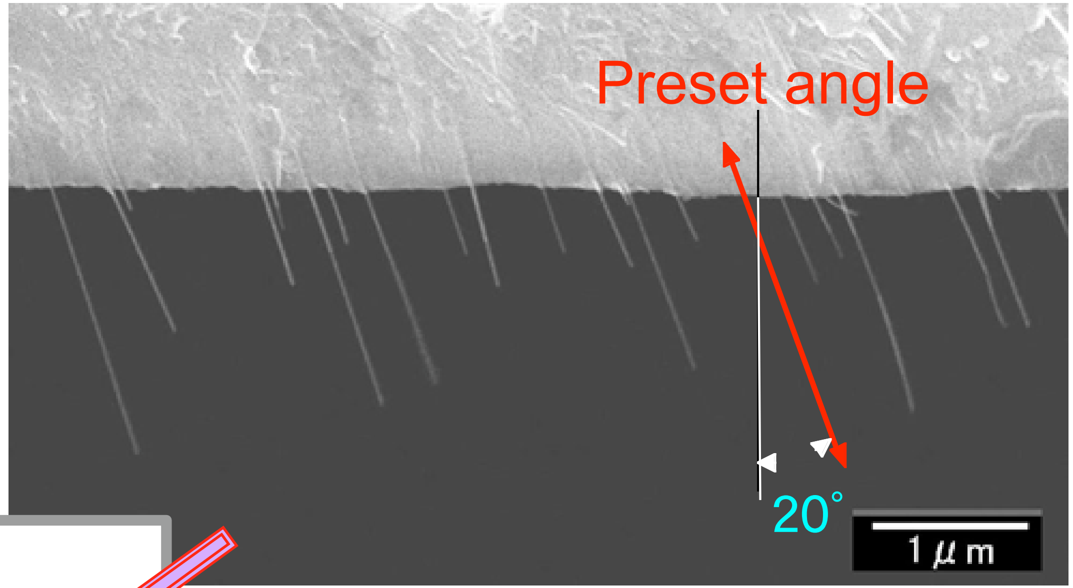
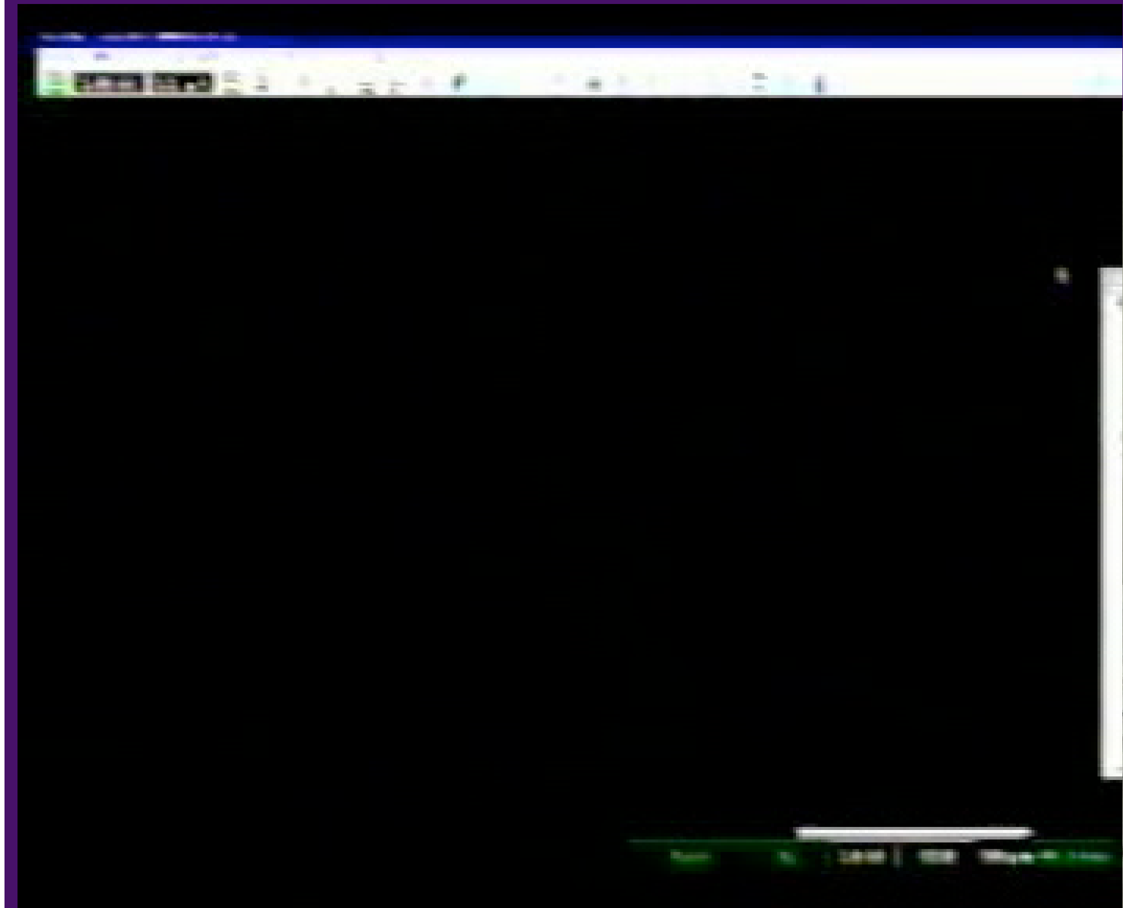
Nanofactory and CNT cartridge





Manipulation of nanotubes in the nanofactory

（from NHK [News ten] 2001/3/23）



Transportation of a nanotube

How robust a nanotube probe is!

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Motivation

CNT
- unique structure (sp[2] bonding)
- excellent electrical & mechanical properties

↓

Building blocks for nanoelectronic devices
nanoelectromechanical systems

Nanoengineering of CNTs such as
gluing, ablation, cutting, layer-peeling, **plastic deformation,** joint formation, etc.

Plastic bend deformation ⟷ Metastable state

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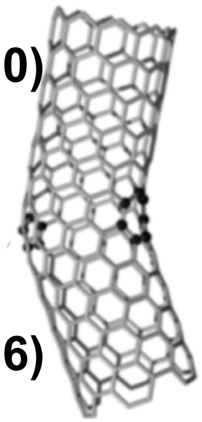
Bending

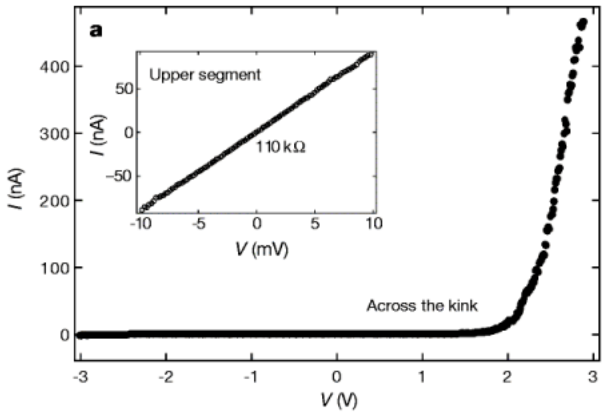
Bend with different chiralities

Electronic devices : M-M,M-S,S-S
Mechanical devices

(9,0)



(6,6)

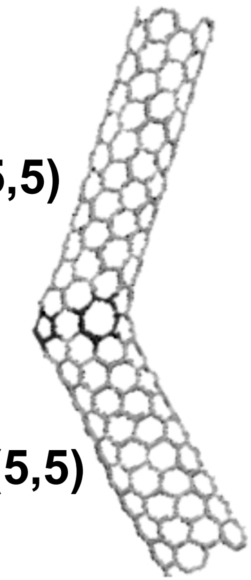


Nature 402,273(1999)

Bend with same chirality

Electronic devices : M-I-M,S-I-S
Mechanical devices

(5,5)



(5,5)

We introduced the plastic bend deformation into a nanotube by current Injection.

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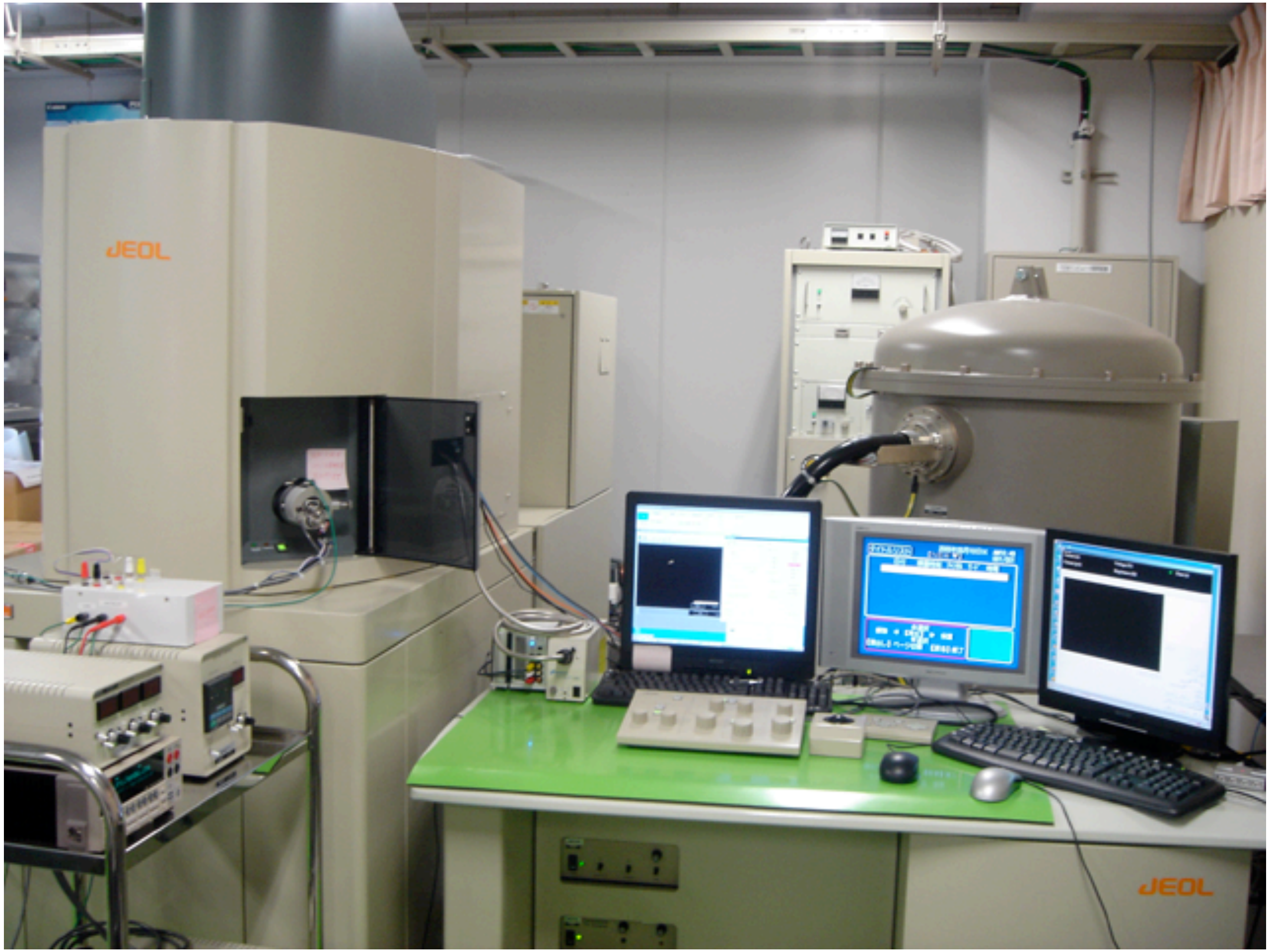
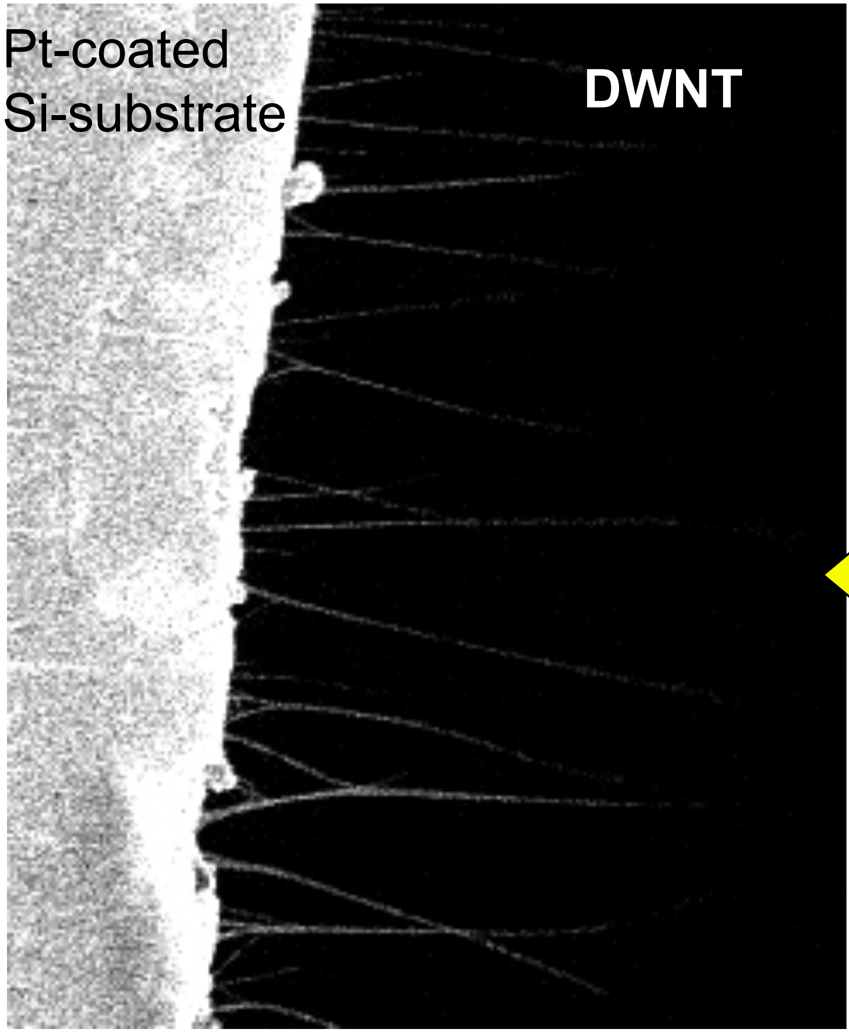
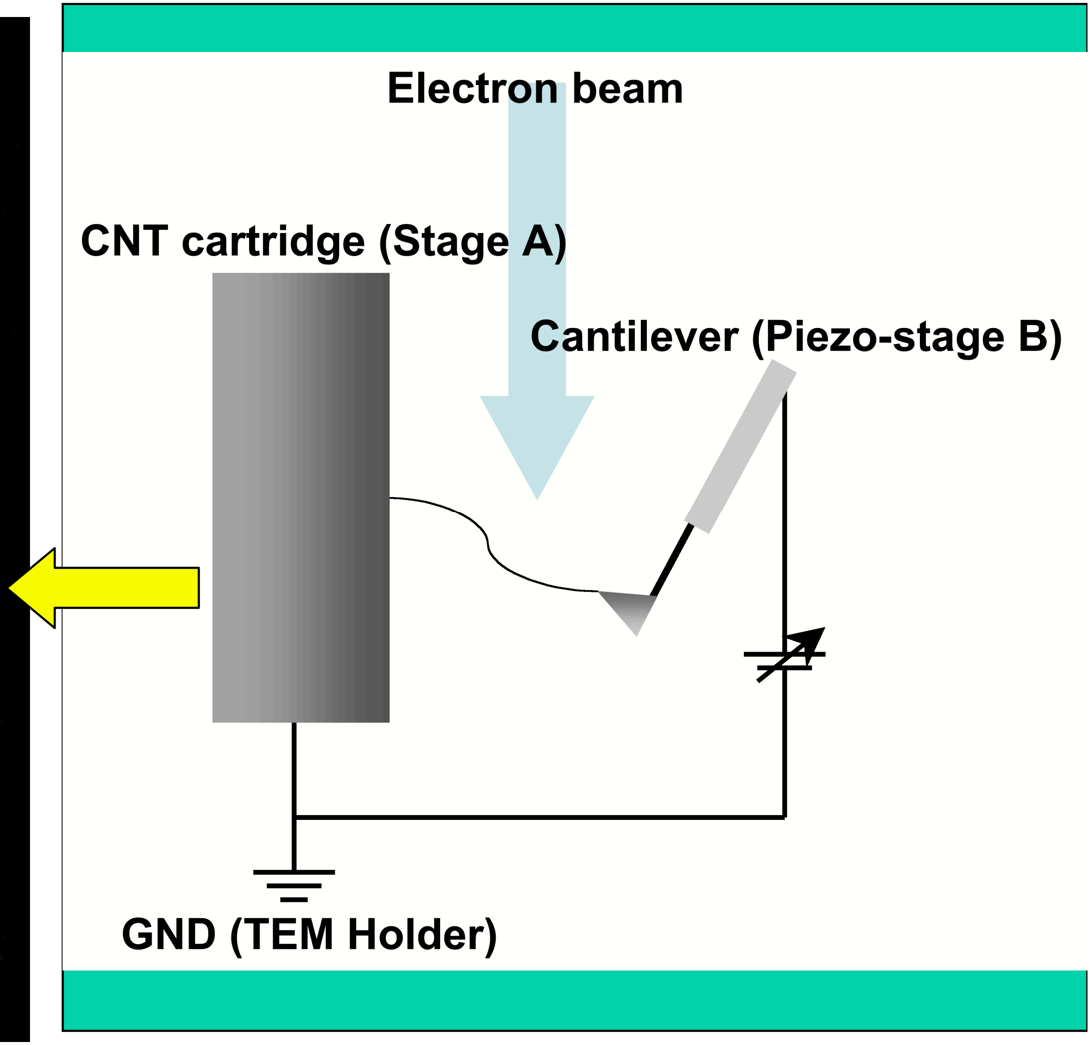
Super-nanofactory and CNT cartridge



Super-nanofactory and CNT cartridge





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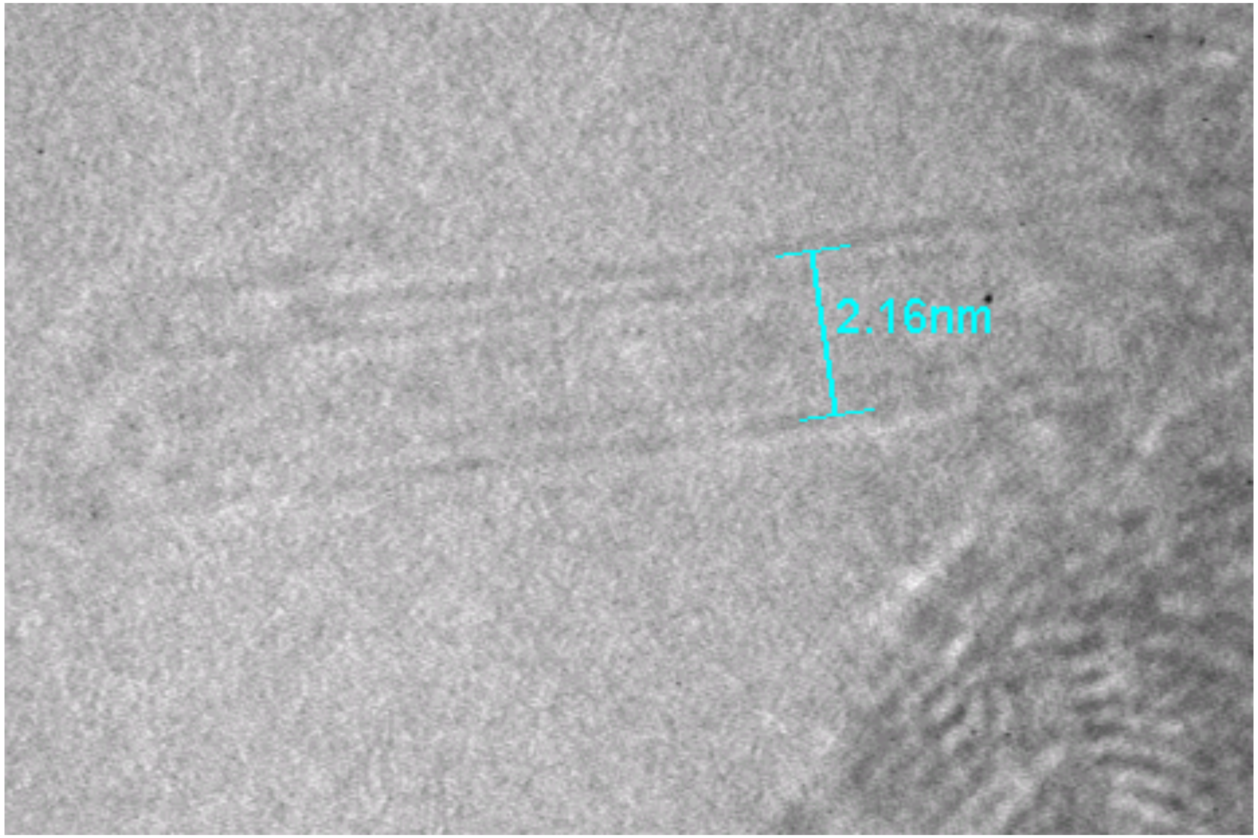
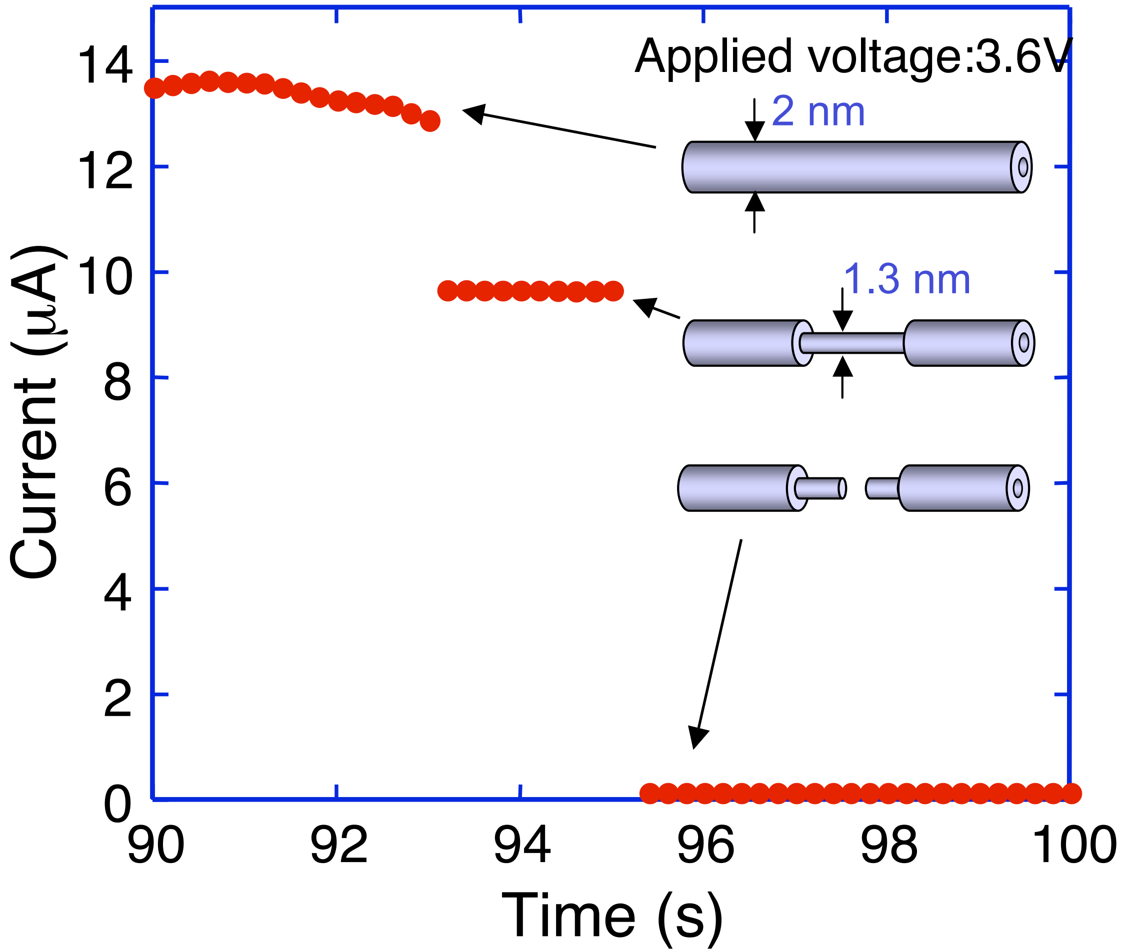
Typical DWNT used in this study

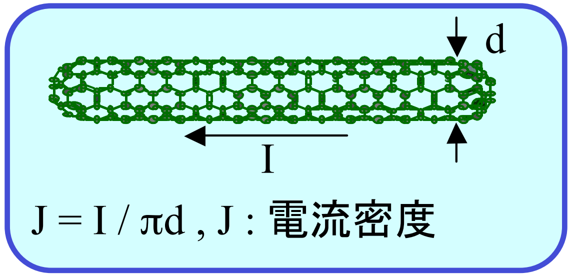


Sublimation current of DWNT



Circumference density of sublimation current J_{so}

J_{S0} = 2.0 μA/nm



〜 2500 K

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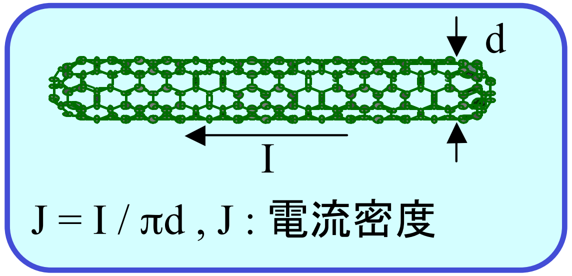
Range of the current examined

☆Current density (J_{S0}) for the **sublimation** of the DWNT

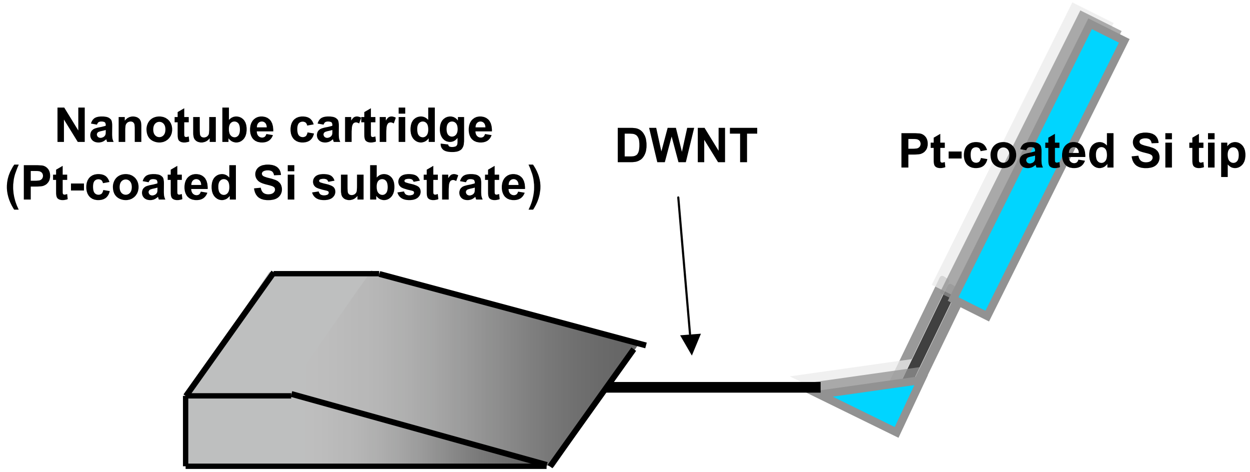
J_{S0} = the Maximum allowable current density

☆Current density(J_{P0}) for the **plastic deformation** of the DWNT

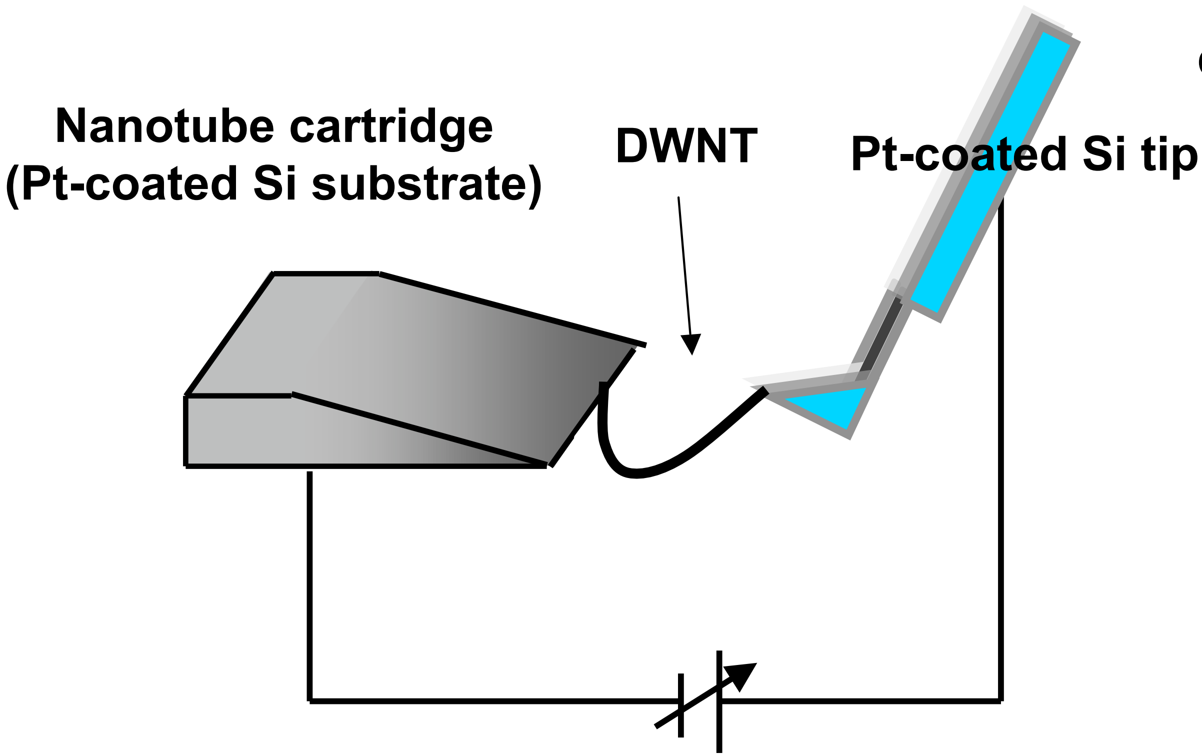
$J_{P0} < J_{S0}$ (2 μA/nm)

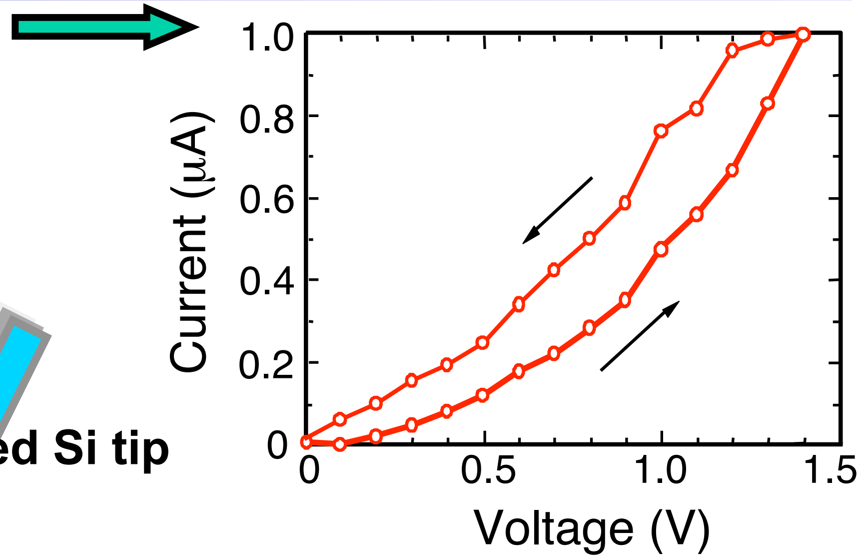


How to induce the plastic deformation



How to induce the plastic deformation





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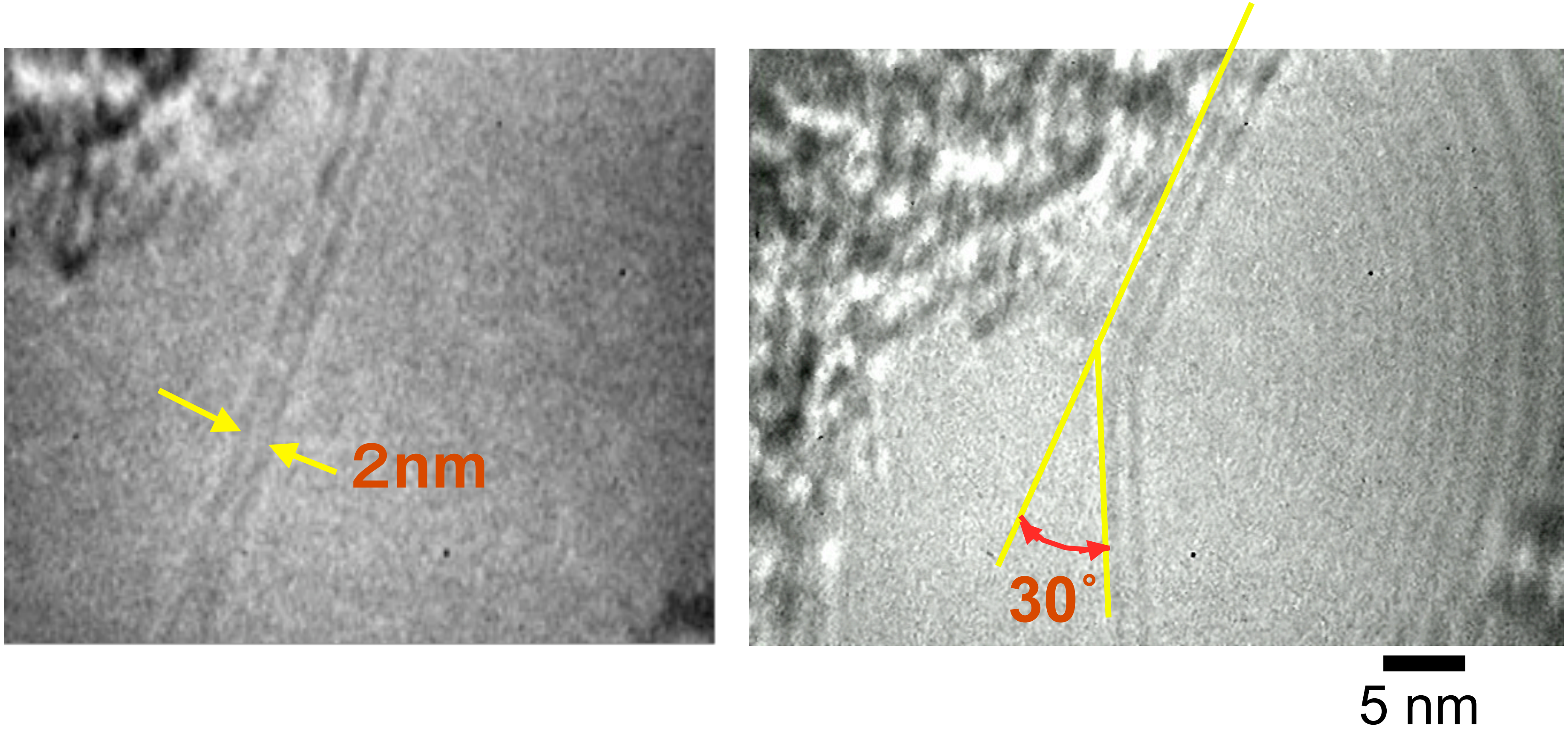
Demonstration of current induced plastic deformation

10nm

Current induced plastic deformation



Y. Nakayama *et al*., Jpn J. Appl. Phys. 44 L720.(2005)

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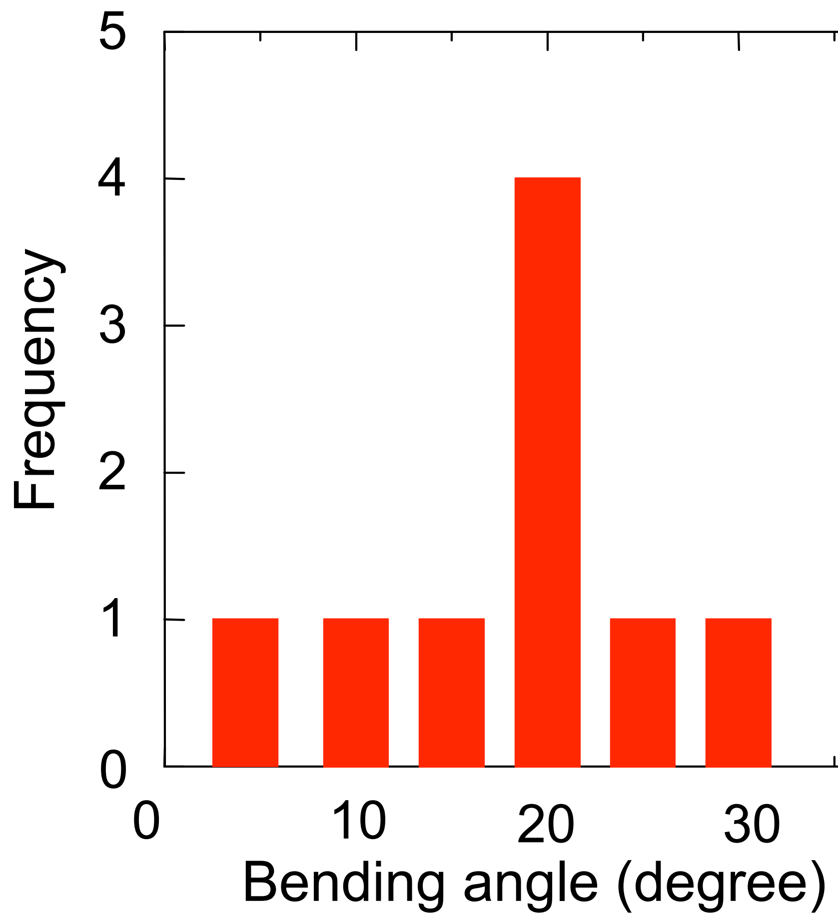
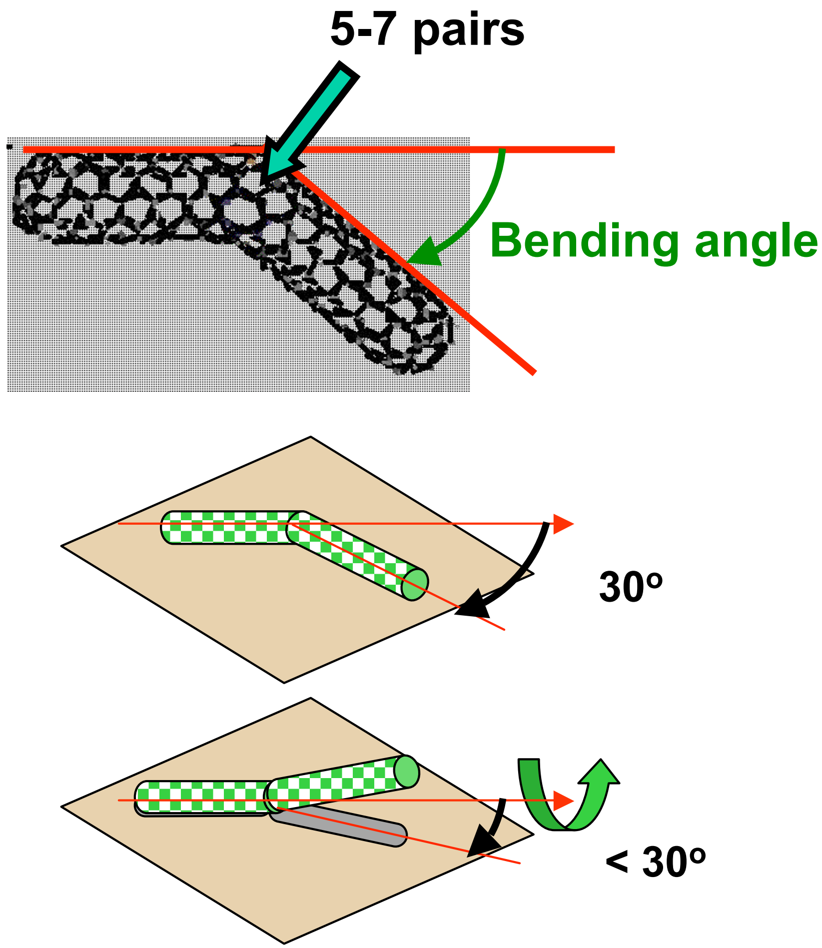
Bending angle of the plastic deformation





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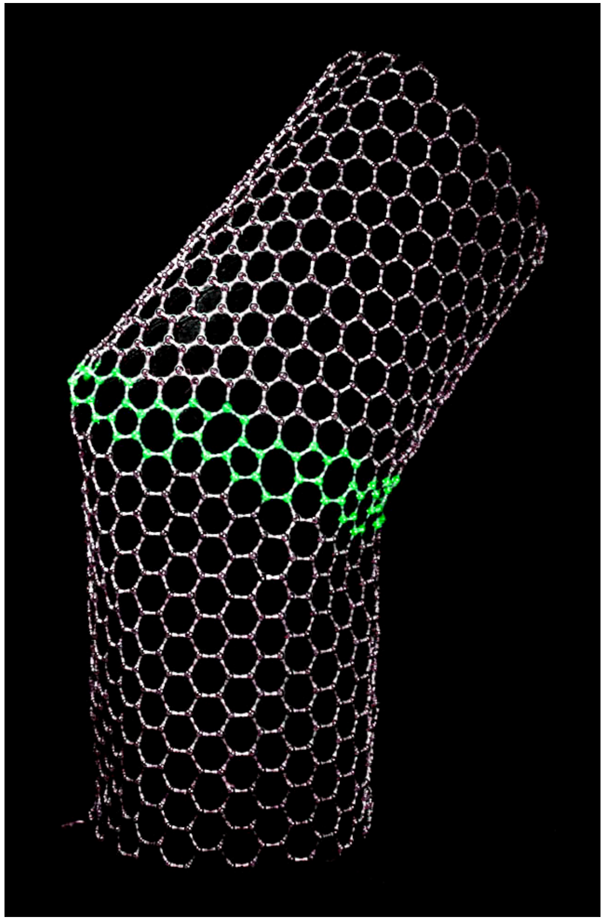
Model for (15,15) nanotube



(15,15) ; ϕ2nm

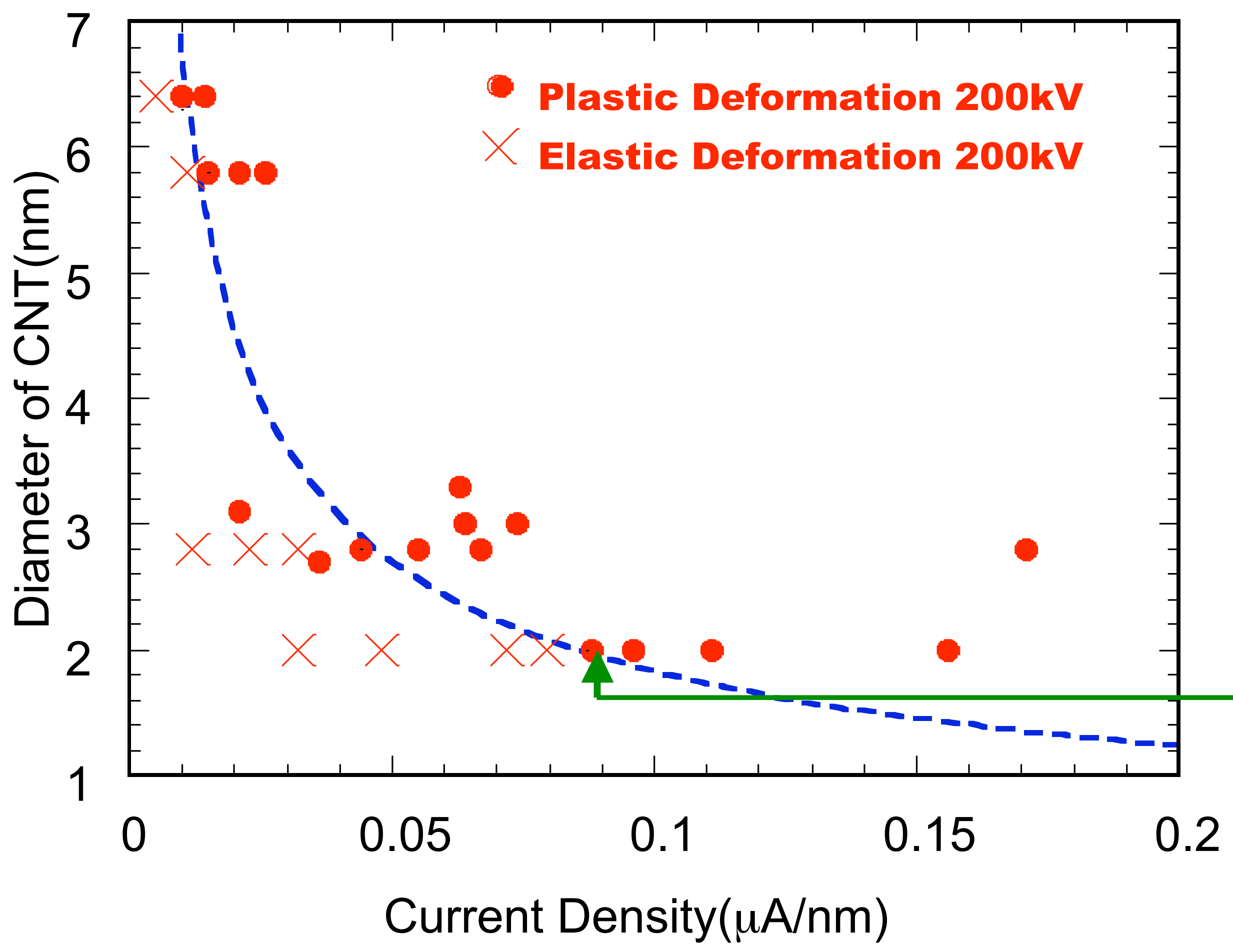
Nanotube of Balls and sticks

~~2 pairs of 5-7 ring~~

14 pairs of 5-7 ring

(with bending angle of 30˚)

Dependence on diameter and electron beam



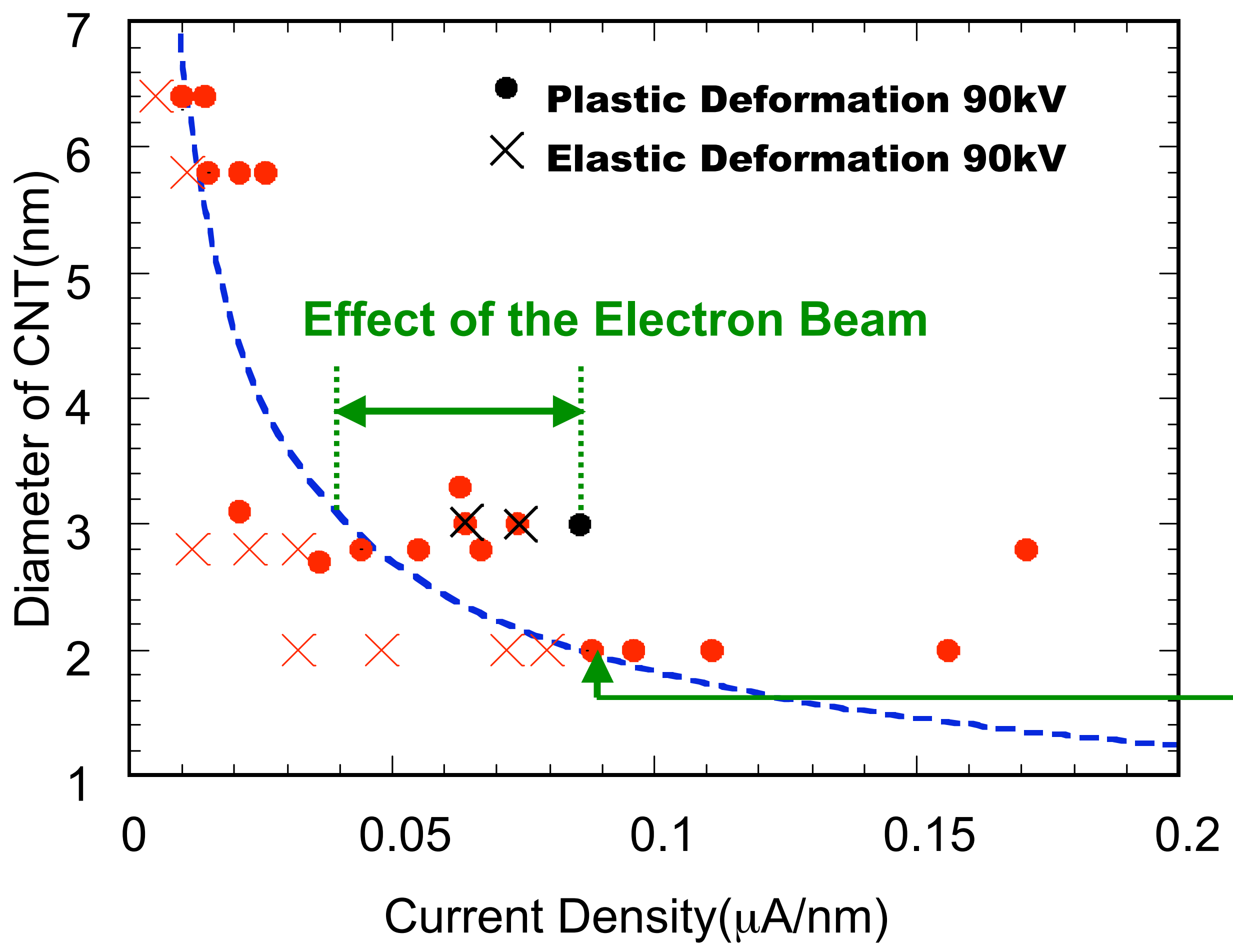
Sublimation

av. 2.2 μA/nm
(φ : 2nm)

Bend Deformation

0.087μA/nm
(φ : 2nm)

Dependence on diameter and electron beam



Sublimation

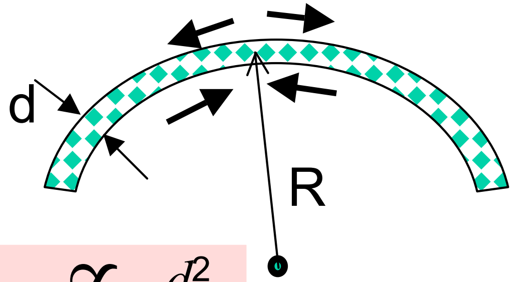
av. 2.2 μA/nm (ϕ : 2nm)

Bend Deformation

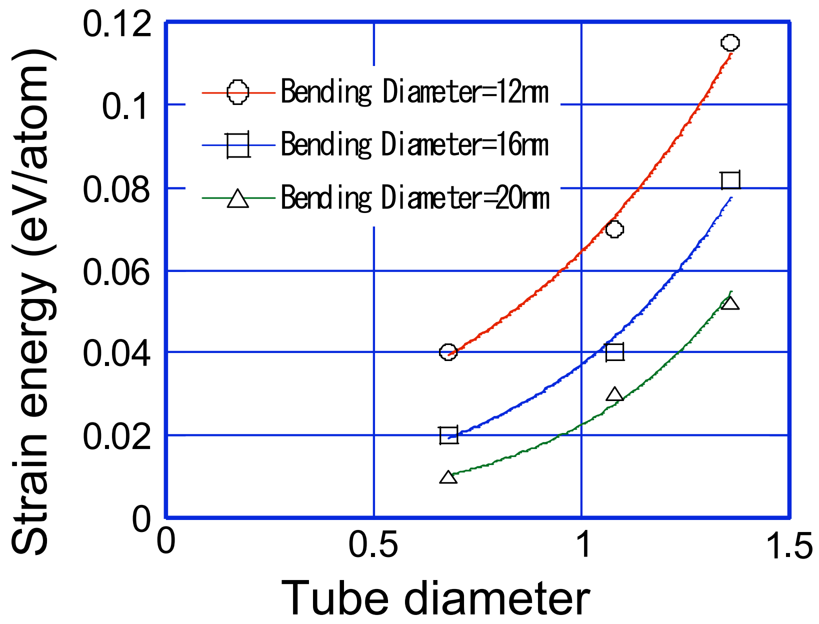
0.087μA/nm (ϕ : 2nm)

Dependence on curvature and diameter

R & d dependence of the strain



Strain $\propto$ d^2

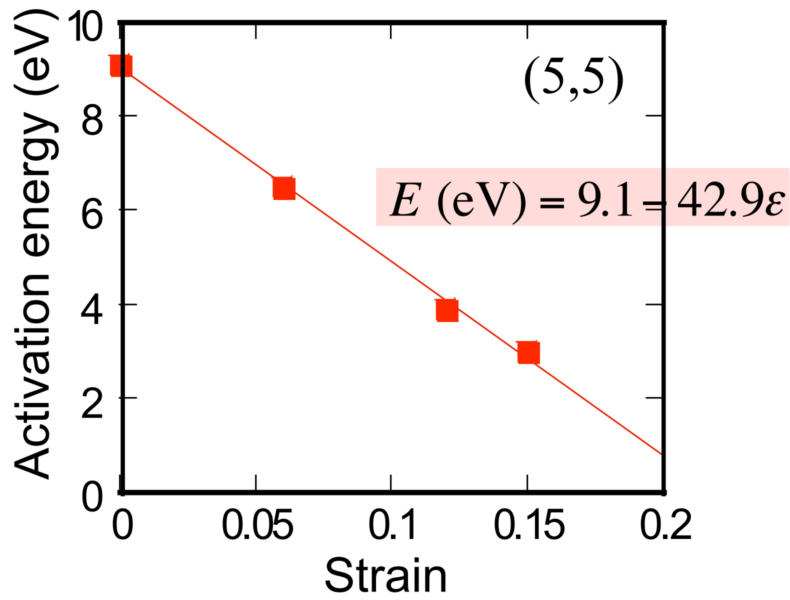


J.Han,Chem.Phys.Let. **282**,187(1998)

Stone-Wales activation energy

$$E = 10.0 - 0.58/d - 17.5\varepsilon$$
$$- 27\varepsilon \sin(2\chi + 46^\circ) \quad [\mathrm{eV}]$$

d: diameter, ε: strain, χ: wrapping angle



T.Dumitrică and B.I.Yacobson,
APL **84**,2775(2004)

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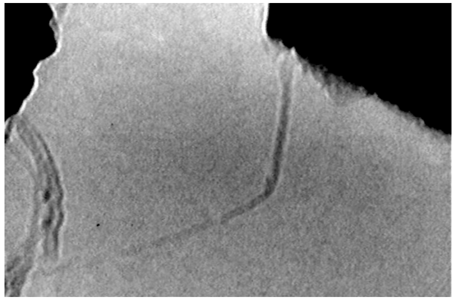
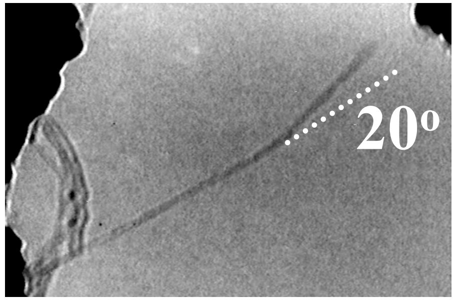
Recovery from bend deformation

Diameter of CNT : 3.3nm

Original shape

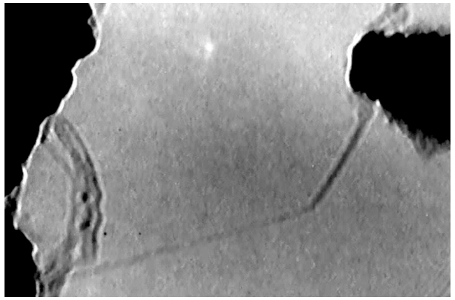


Current under duress



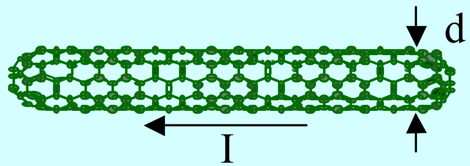
Permanent bend

0.06μA/nm



Contact with the Si tip again

Applying more current to the bend portion



$J = I / \pi d$, J : 電流密度

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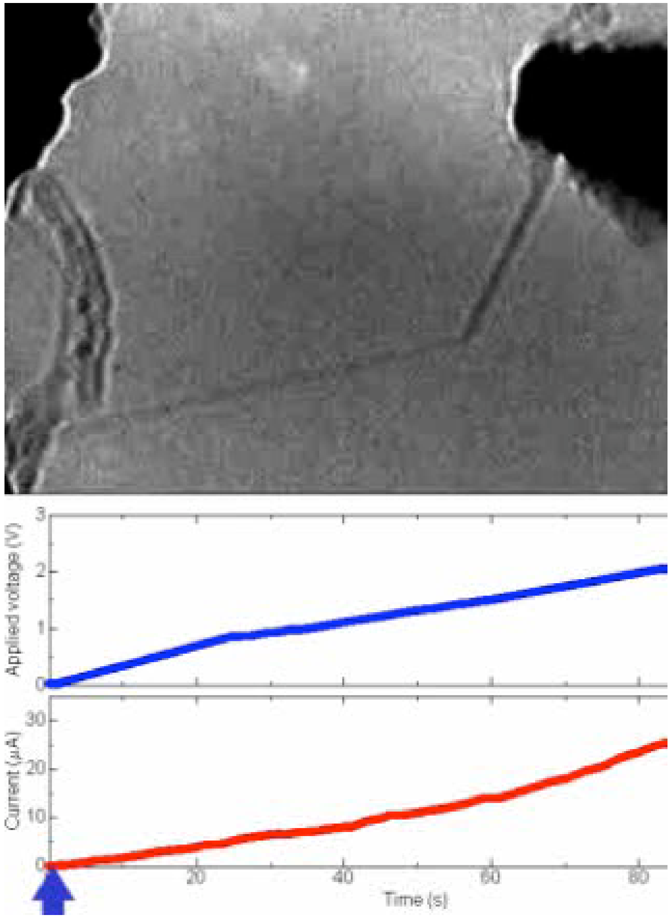
Demonstration of recovery from bend deformation

Diameter of CNT : 3.3nm



Voltage

Current

At 3.2μA/nm the CNT becomes straight

3.2μA/nm is close to the sublimation current for this CNT

The sublimation temp.

∽2500K

X. Cai, S. Akita and Y. Nakayama, Thin Solid Films 464-465, 364 (2004).

This recovery apparently results from the curing of defects of pentagon–heptagon pairs at∽2500K

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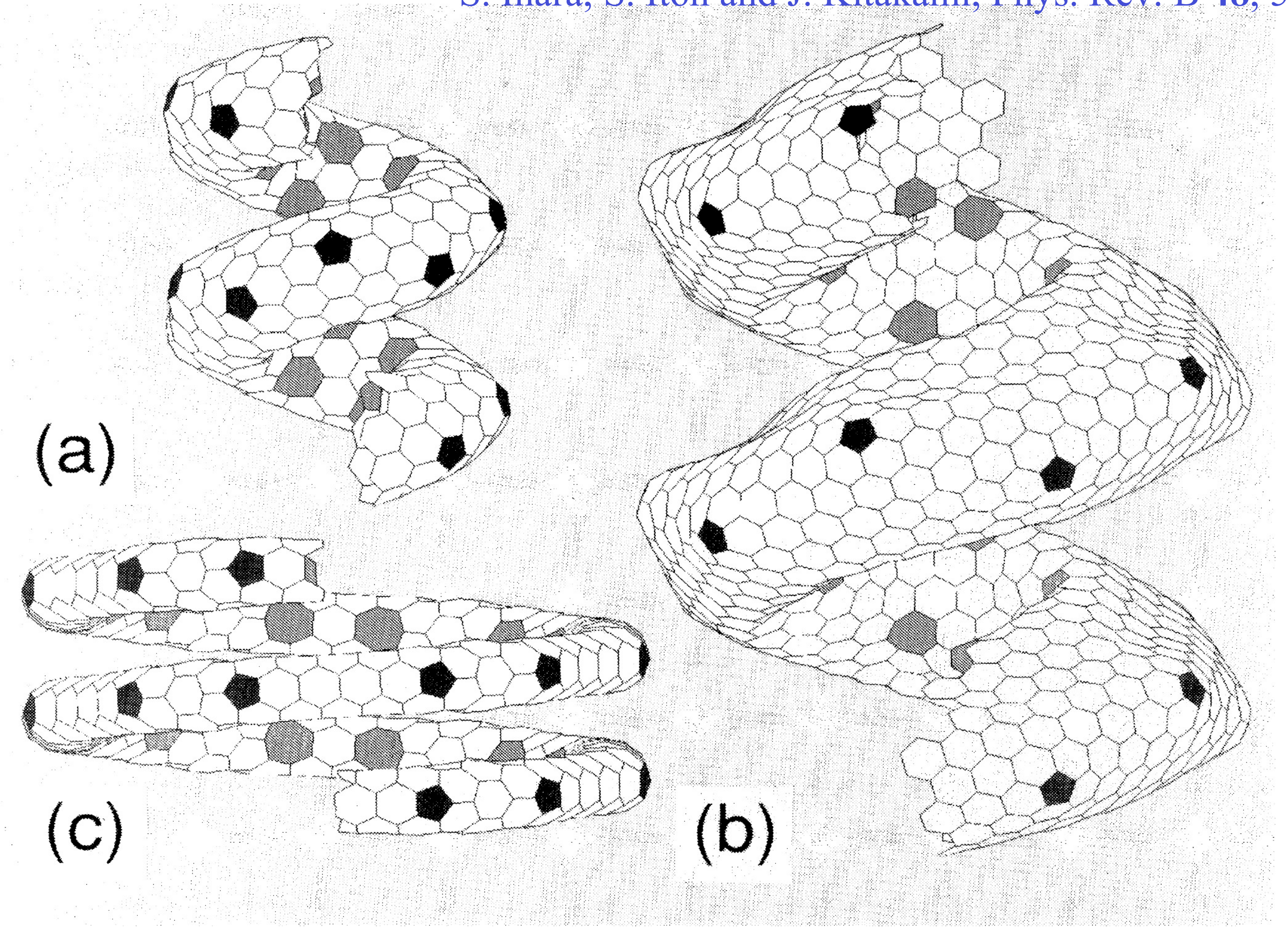
Confirmation of universality of curing phenomena

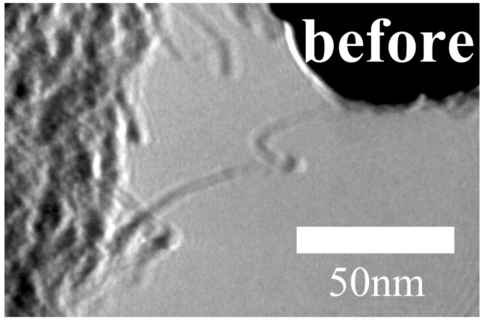
S. Ihara, S. Itoh and J. Kitakami, Phys. Rev. B **48**, 5643 (1993).

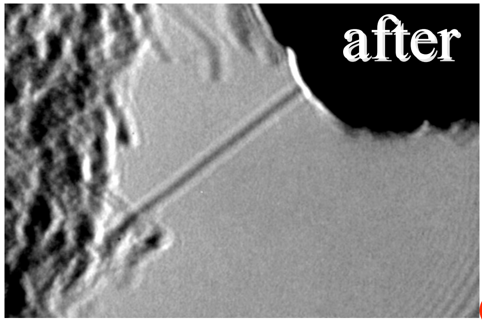


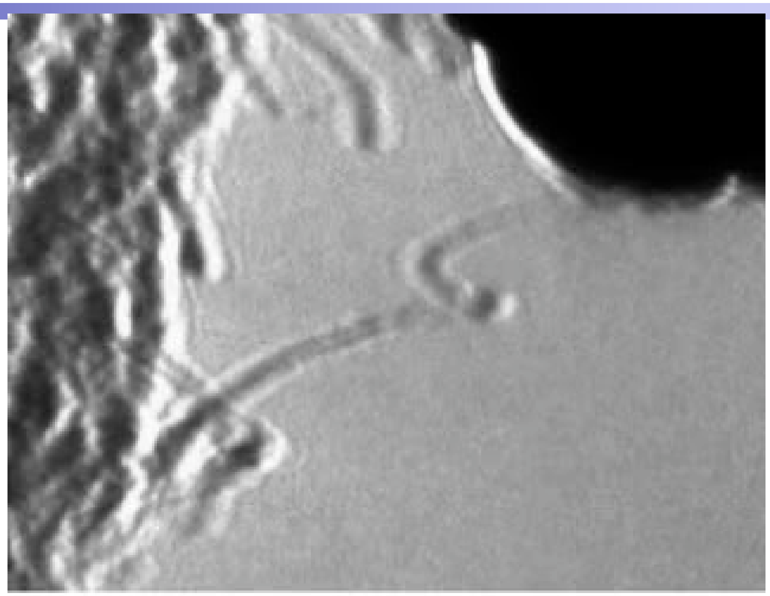
Coils have pentagons and heptagons, respectively, in the outer and inner ridgelines. ➡ Good example

Demonstration of recover from helical

Diameter of CNT : 3.7nm

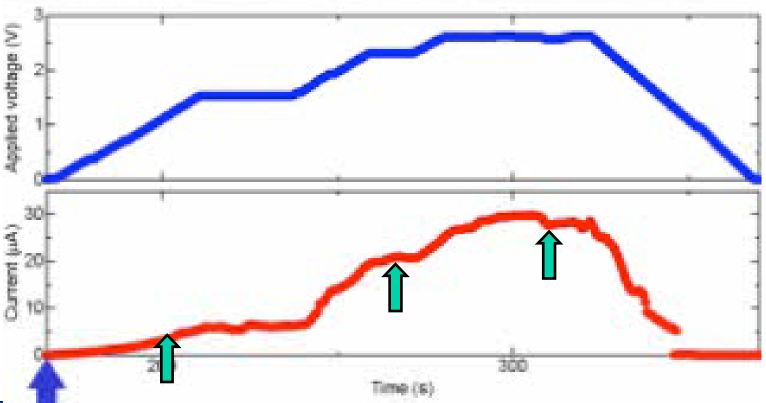


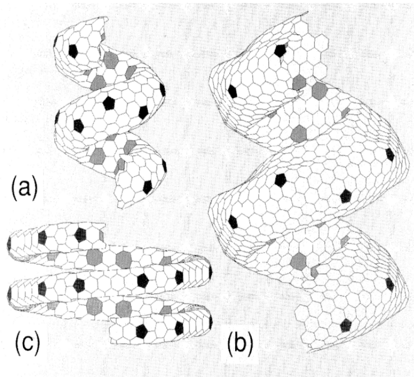




Voltage

Current





S. Ihara, S. Itoh and J. Kitakami, Phys. Rev. B **48**, 5643 (1993).

The coil started to loosen at 0.9 μA/nm, drastically changed its structure at 2.2 μA/nm and became straight at 2.6 μA/nm.

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(SEM with manipulator)

◎ Plastic deformation of CNT

・Manipluration in Supernanofactory (TEM with manipulator)

◎ Recovery from the plastic-deformation

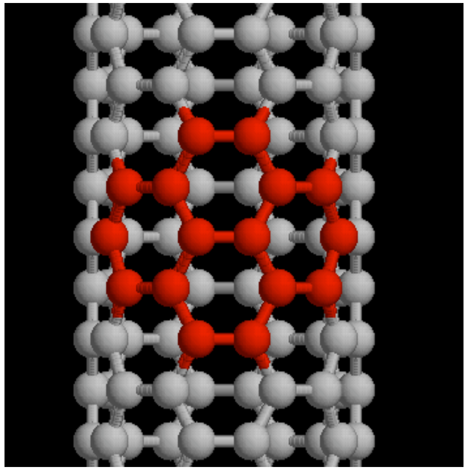
◎ Computer simulation

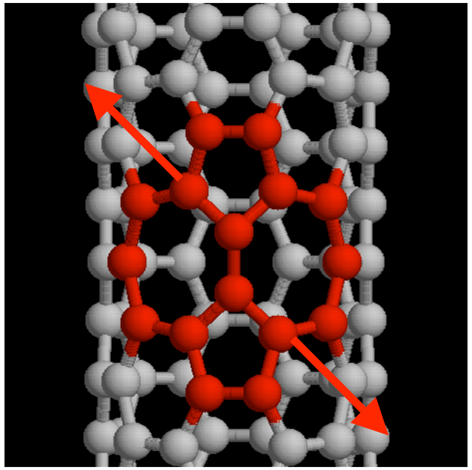
・Potential barriers for the plastic-deformation

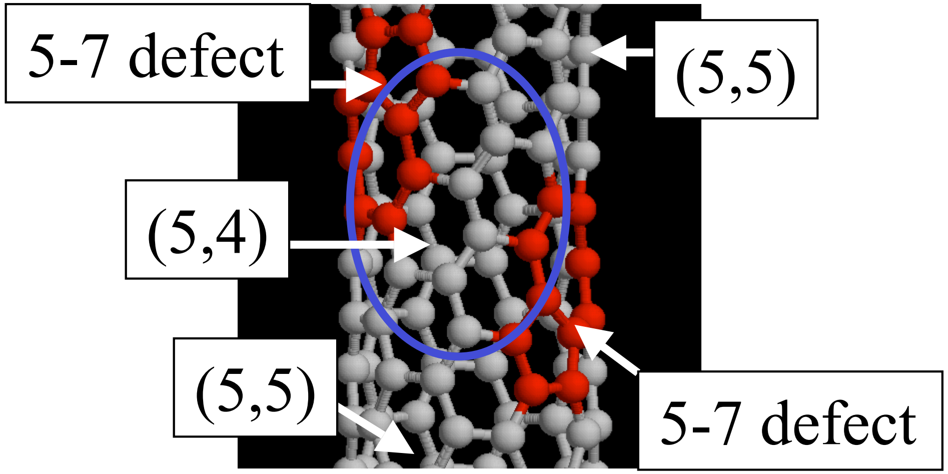
◎ Conclusion

Ductile model of SWNT

(5,5)







Nucleation
of
Stone-Wales defect

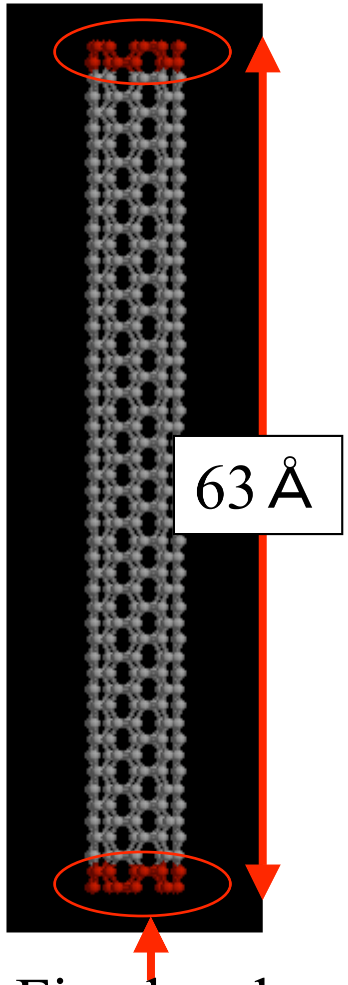
Splitting
of
5-7 defect

For obtaining activation & formation energies of defects

Test model:
(5,5) 63 Å 520 atoms
(8,0) 63 Å 480 atoms

Boundary condition:
- Fix end.
- Others are free.

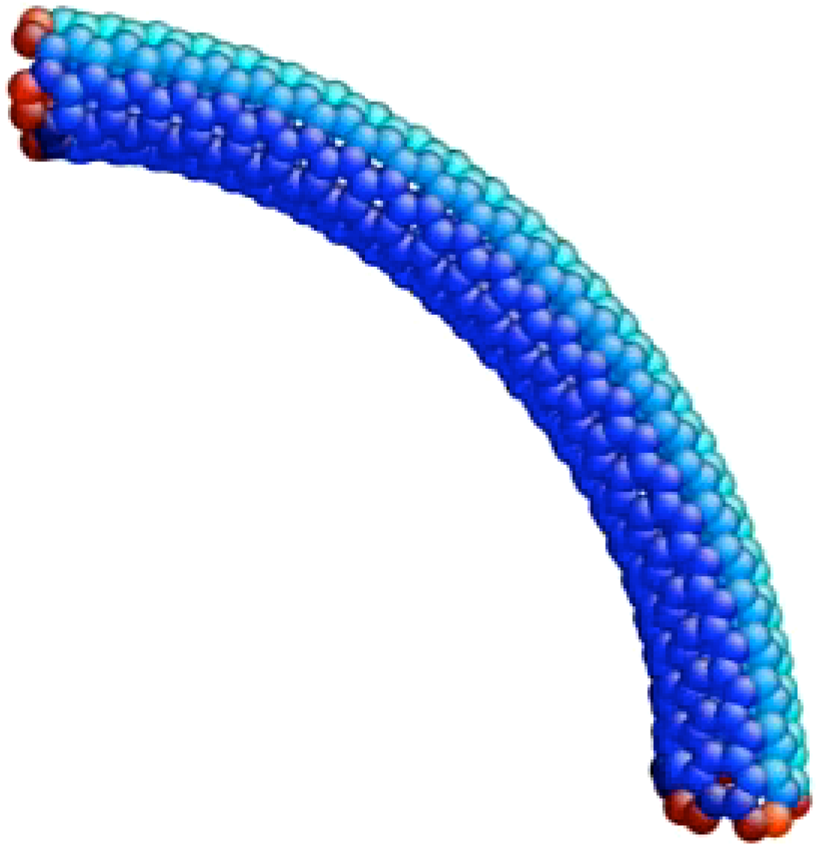
Test potential:
Classical type.

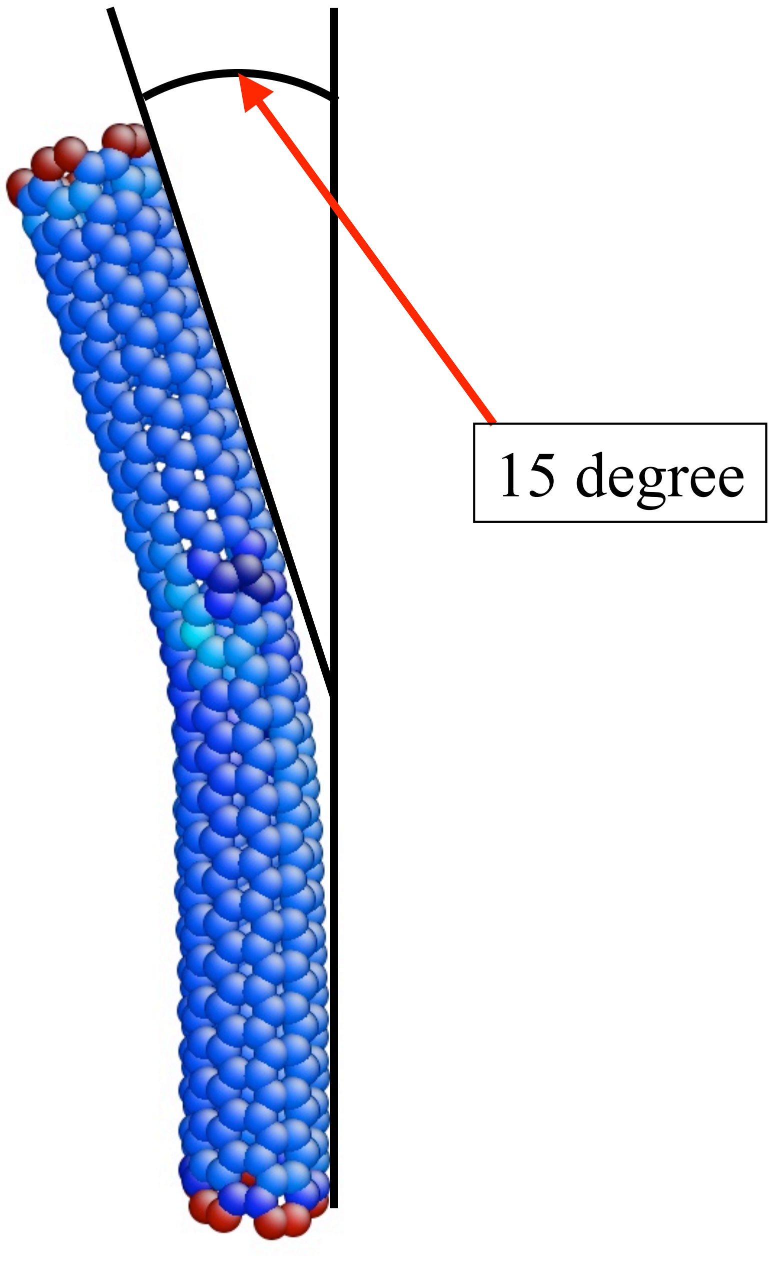


Fixed end

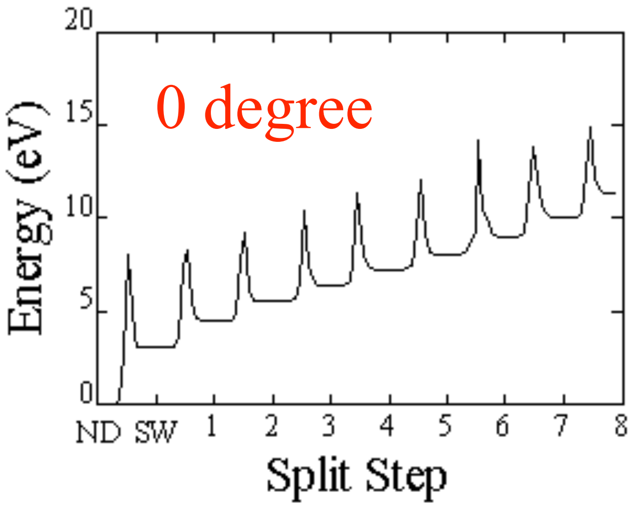
Simulation Step

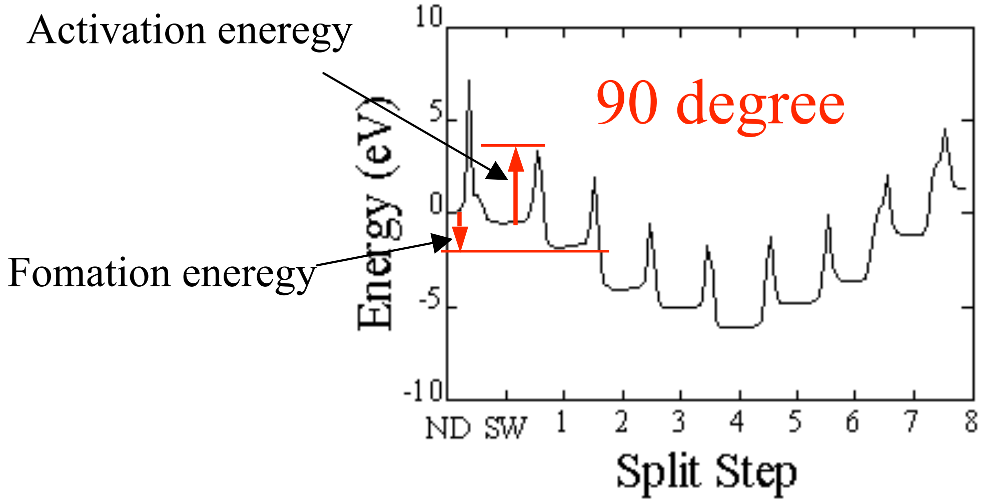
1. Optimization of non defect model
2. Introduction of S-W defect
3. Optimization of S-W defect model
4. Splitting S-W defect into two 5-7 pairs
5. Optimization of split model
6. Walk of 5-7 pairs
7. Optimization of split model
8. Repeat of 5, 6 steps

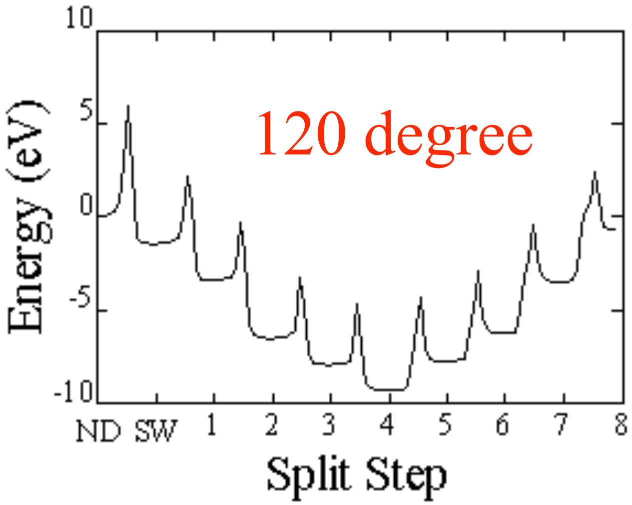


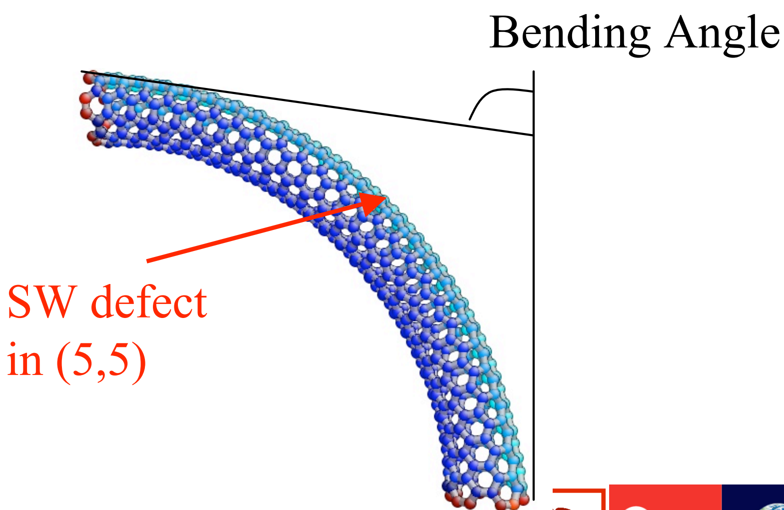

15 degree

Activation & formation energies of defects for (5,5) SWNT





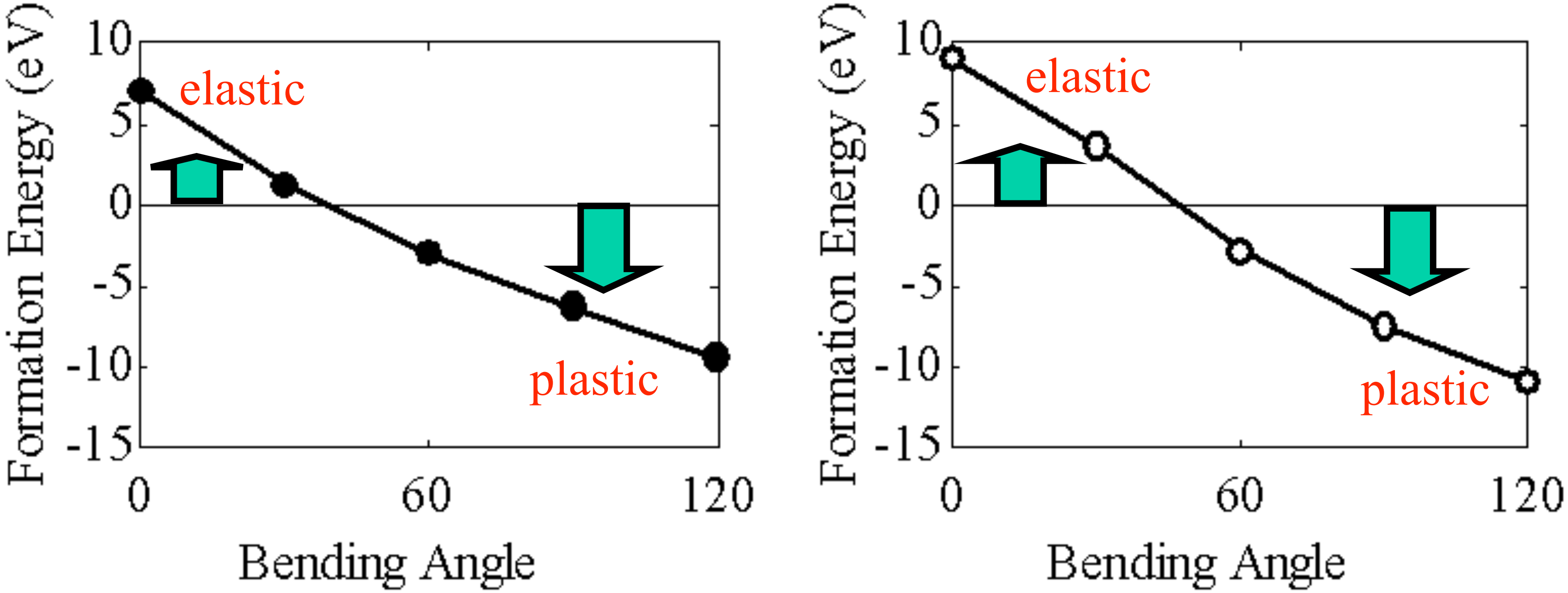




Prefecture
University

Formation energies of bond rotations

(5,5) (8,0)



Bending angle > 50° is required for forming plastic bend deformation.

Osaka Prefecture University

Frequency of bond rotations

Temperature and Time dependence of plastic deformation

Arrenius equation

$$f = \nu \exp\left(-\frac{E_{\mathrm{act}}}{k_{\mathrm{B}}T}\right)$$

k_B :Boltzmann constant

$\nu = 10^{13}\ \mathrm{s}^{-1}$

$T = 1500\mathrm{K}$

$E_{act} = 4\ \mathrm{eV}$

↓

$f = 0.33\ \mathrm{s}^{-1}$

↓

Bond rotation occurs within a few seconds

Outline

◎ What is a carbon nanotube (CNT) ?

◎ Manipulation of CNT in Nanofactory

(SEM with manipulator)

◎ Plastic deformation of CNT

・Manipluration in Supernanofactory (TEM with manipulator)

◎ Recovery from the plastic-deformation

◎ Computer simulation

・Potential barriers for the plastic-deformation

◎ **Conclusion**

Conclusion

From Experiment

(1) The bending **angles** are in the range of **20-30°.**
The bend consists of 5-7 rings.

(2) The onset **Current Density** for the permanent bend was measured less than **1/20** of that for the sublimation.

(3) Plastic bend is **metastable:** it recovers at the current density **close to the sublimation one**.

From Simulation

(4) Both **thermal energy** and **mechanical duress** are necessary for the **plastic deformation**.

(5) The **energy barrier** for plastic deformation and recovery ranges from **3.6 to 6.0 eV,** depending on the chirality.