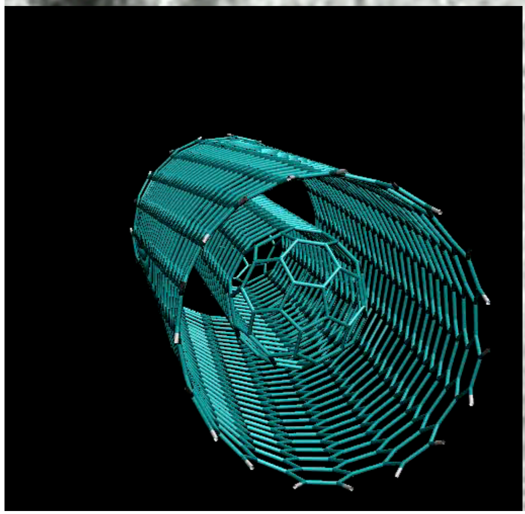
NT'06 Conference
June 18-23, 2006
Hotel Metropolitan Nagano

Current-Induced Reversible Deformation of Carbon Nanotubes

Y. Nakayama[1,2)]

[1)]Osaka Prefecture University

[2)]Osaka University



Acknowledgements

Ms. A. Nagataki (Osaka University)

Dr. O. Suekane (Osaka Science & Technology Center)

Mr. H. Mori (Osaka Prefecture University)

Prof. S. Ogata (Osaka University)

Prof. J. Li (Ohio State University)

Prof. S. Akita (Osaka Prefecture University)

Osaka Prefecture University

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Outline

1 Brief introduction of our research activity on nanocarbon and also of nanocarbon project

2 Reversible deformation of CNT

2-1 Plastic deformation of CNT

- Manipluration in Supernanofactory (TEM with manipulator)
- Plastic deformation

2-2 Recovery from the plastic deformation

2-3 Energetic analysis of plastic bending

- Nudged elastic band minimum energy path calculation with a bond-order potential

3 Summary

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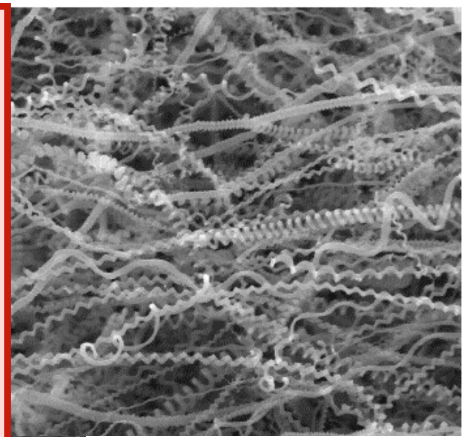
1. C

Recent progress in Growth process of unique CNTs

/ Large-scale CVD process of CNT
/ Long CNT growth ----------------- (A007)
/ Function of catalysts for CNCs --- (B027)
/ Effective catalysts for CNCs ------ (B021, B026)
/ ----- etc.



/ High rate growth of CNTs

2. Na

Recent progress in Nanoengineering of CNTs

/ Plastic deformation ------------ (1003, D053)
/ Recover from deformation ---- (1003)
/ Junction formation ------------- (E060)
/ Mechanical strength ----------- (E054, E056)
/ Electric contact ----------------- (F016)
/ Piezo gate CNT-TFT ---------- (G016)
/ Probe for a bio-molecule ----- (C030)
/ Field emission ------------------ (F034)
/ Alignment of CNC ------------- (D069)
/ ----- etc.

/ ----------

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Tip

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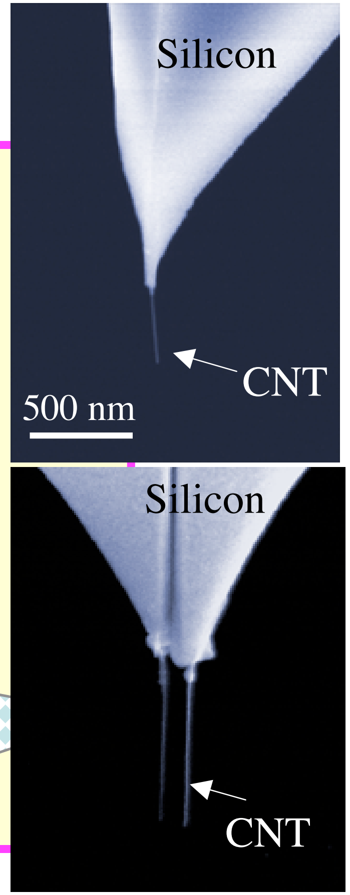


Project of CREATE Osaka:

"Development of application techniques for nanocarbon materials"

Sponsor: Japan Science & Technology Agency (JST)

Organization: Collaboration of Regional Entities for the Advancement of Technological Excellence (CREATE)

Dispenser: Osaka Prefecture

Core Labs：Tech. Res. Inst. of Osaka

Jan. 2005 ～ Dec. 2009

- 3 universiti…
- 2 res… …tutes
- …

CREATE OSAKA

JST大阪府地域結集型共同研究事業

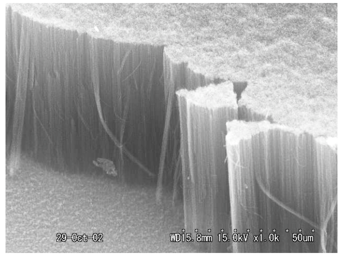
Osaka Prefecture Project : (2005〜2009)

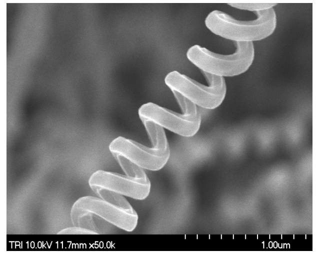
“Development of application techniques for nanocarbon materials”

Theme 1 : Development of large-scale synthesis of unique nanocarbon materials

1-1 Brush-type carbon nanotubes

1-2 Carbon nanocoils





Theme 2 : Development of highly functional materials using brush-type carbon nanotubes

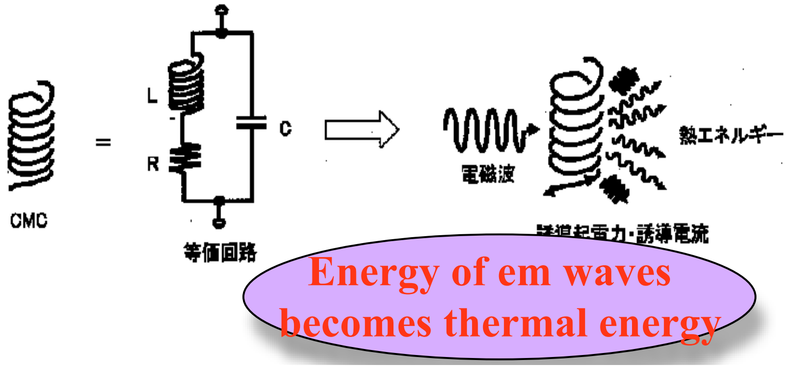
2-1 High strength fibers, ropes, sheets

2-2 Super capacitor devices

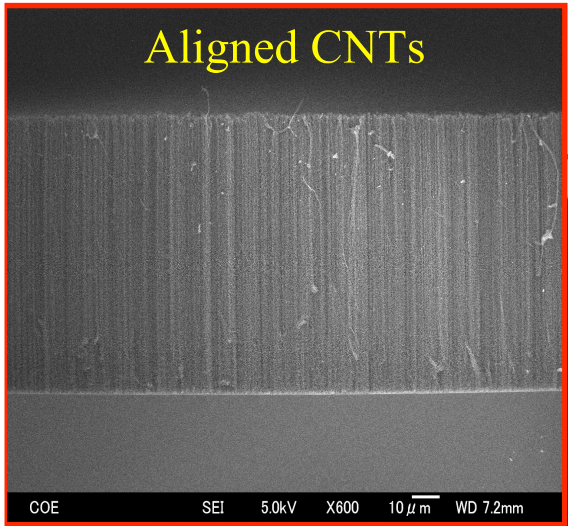
Theme 3 : Development of highly functional materials using carbon nanocoils

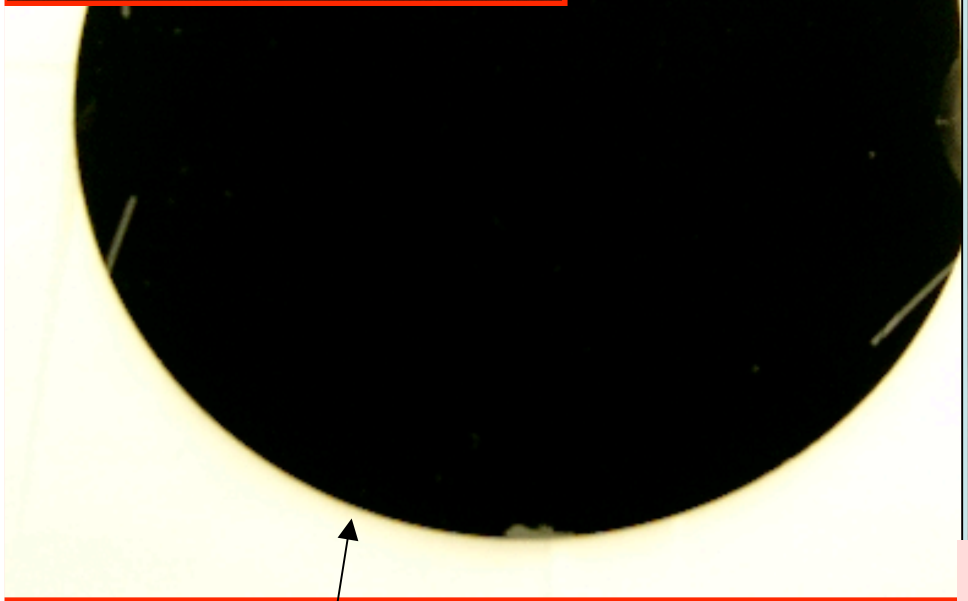
3-1 Highly functional compounds

3-2 Electromagnetic wave absorber



Large-scale deposition of brush-type carbon nanotubes

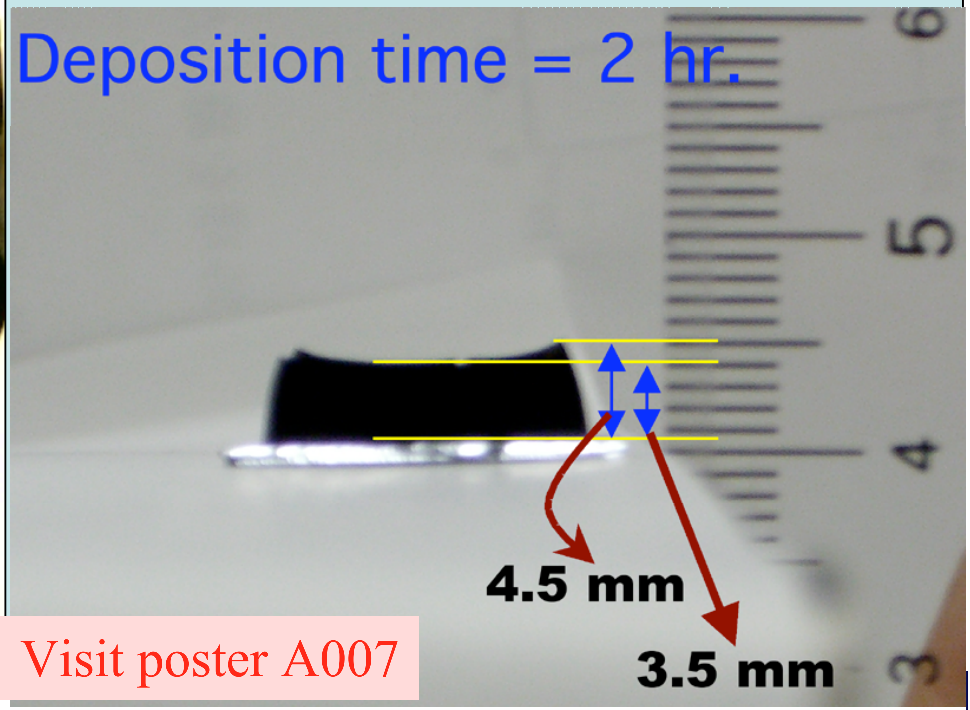




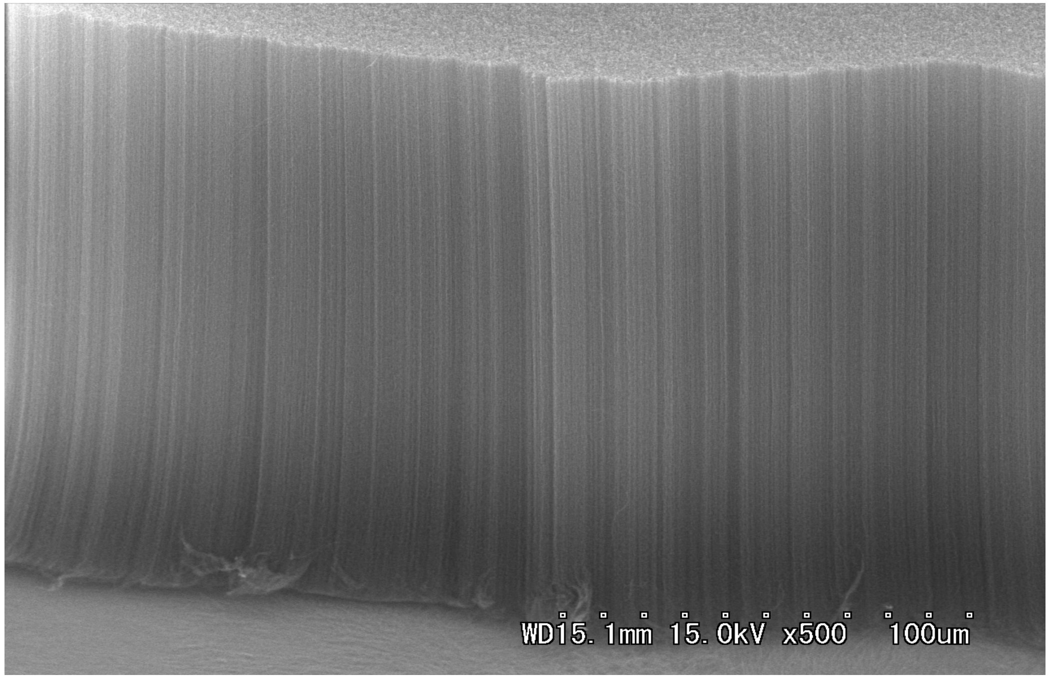
Brush-type CNTs grown on a large-sized Si wafer

1. Development of a system for large-scale synthesis
2. Synthesis of long brush type of CNT (CNT3.5mm)

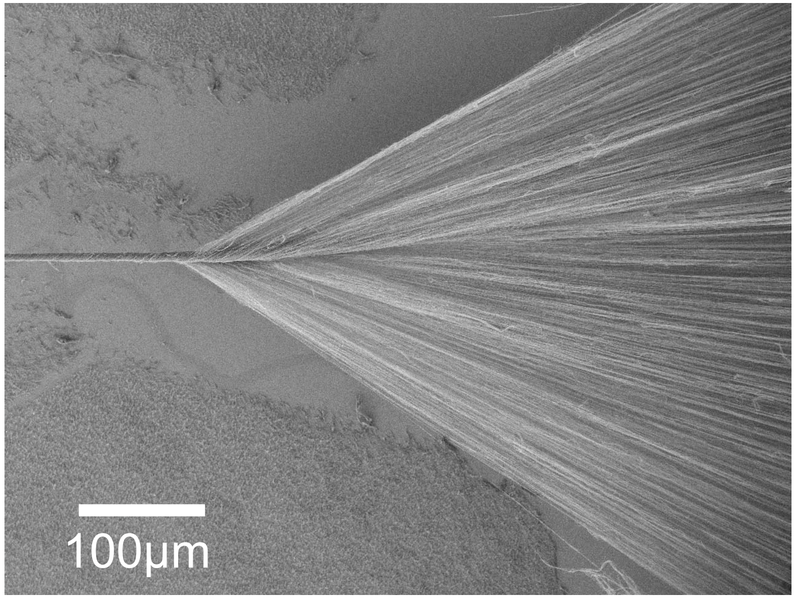
Photograph of 3.5 mm long CNTs



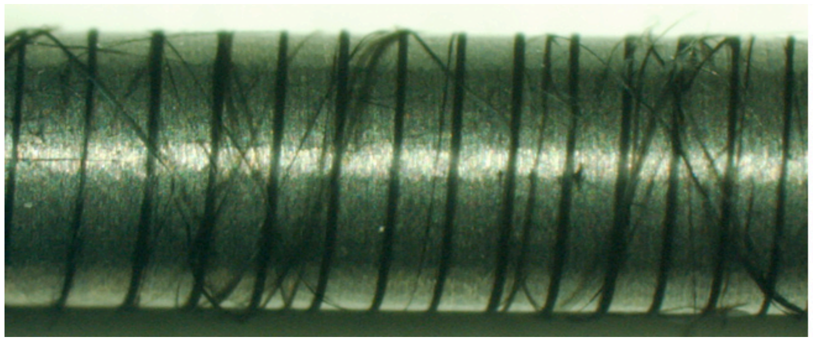
Development of high strength fibers. ropes, sheets using CNTs



Brush-type of CNTs



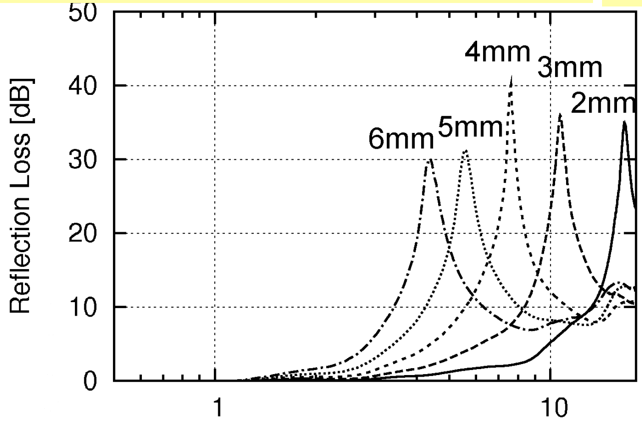
Drawing and spinning a yarn (x200)



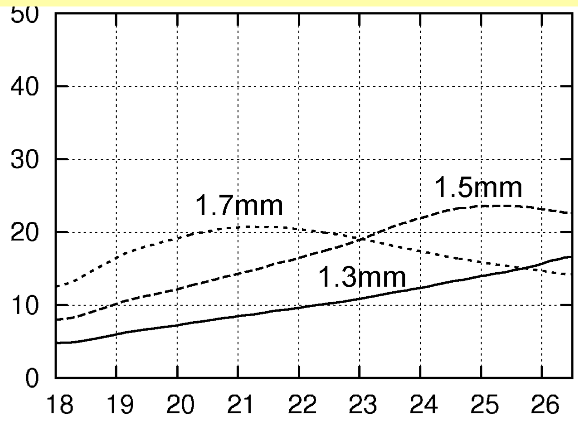
CNT yarn rolled up

Development of em absorbers

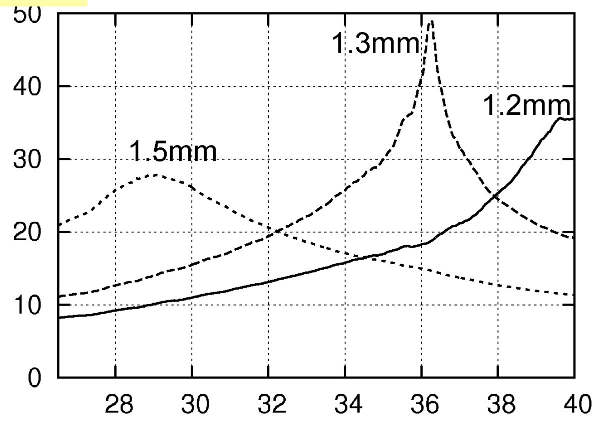
Compound with 5wt% CNC (tunable and more than 20dB)



0.5～18GHz

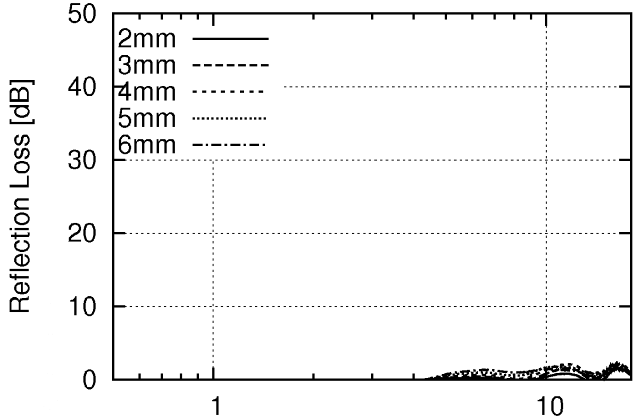


18～26.5GHz

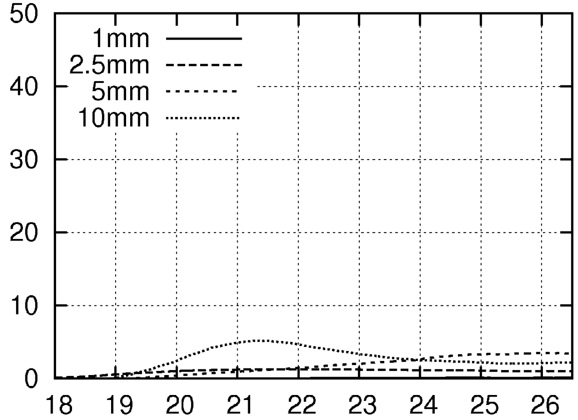


26.5～40GHz

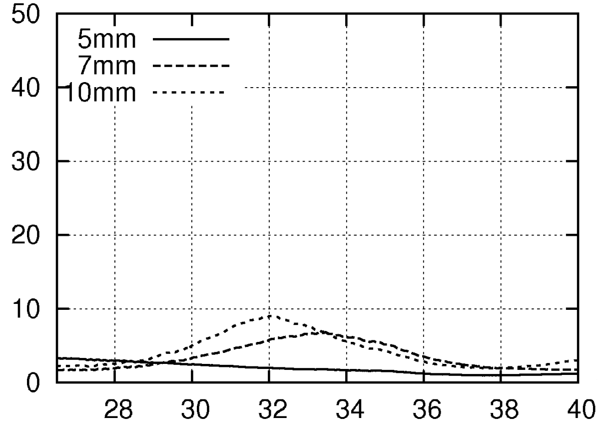
Compound with 5wt% CB (less than 10dB)



0.5～18GHz



18～26.5GHz



26.5～40GHz

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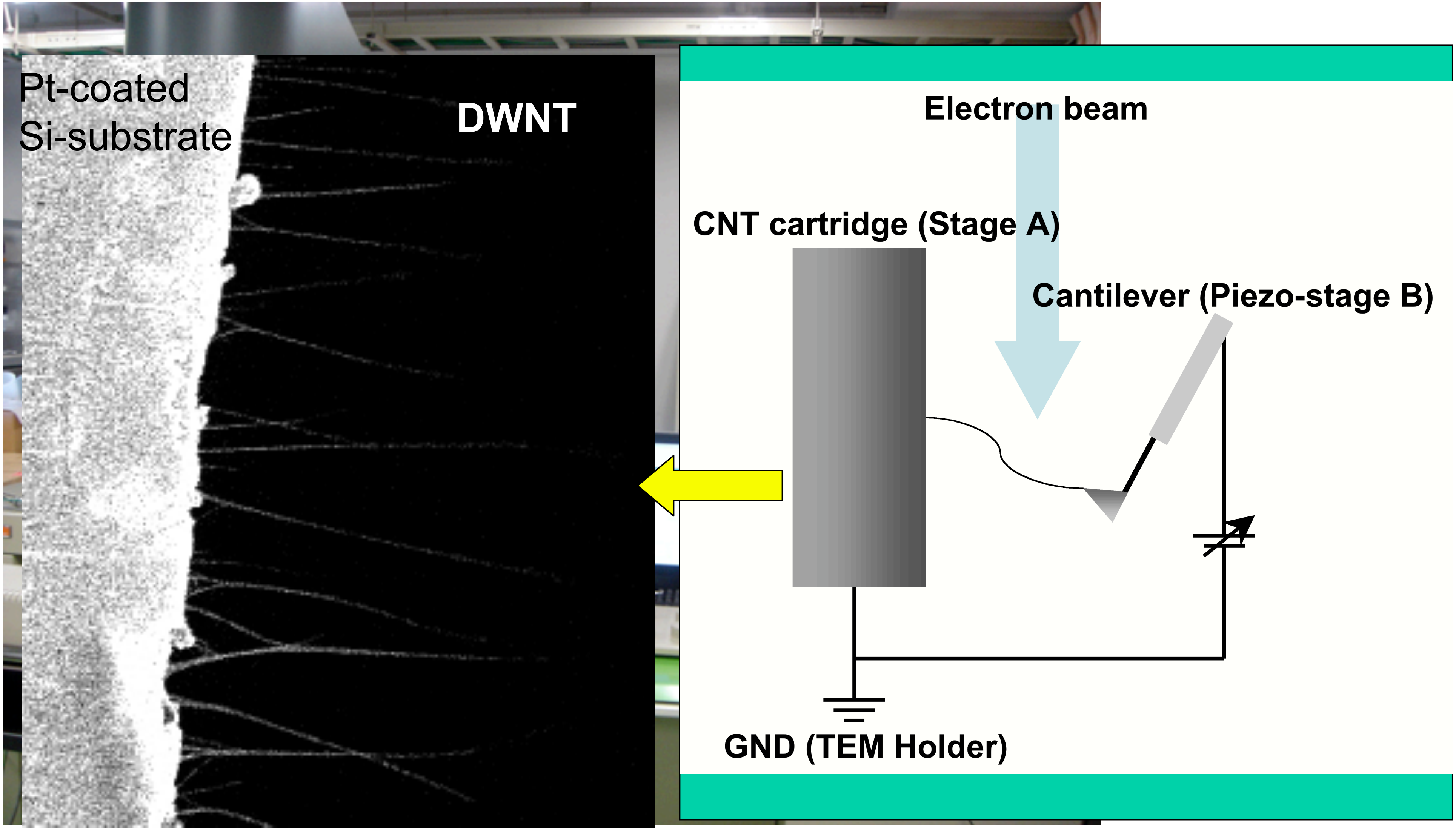
Super-nanofactory and CNT cartridge



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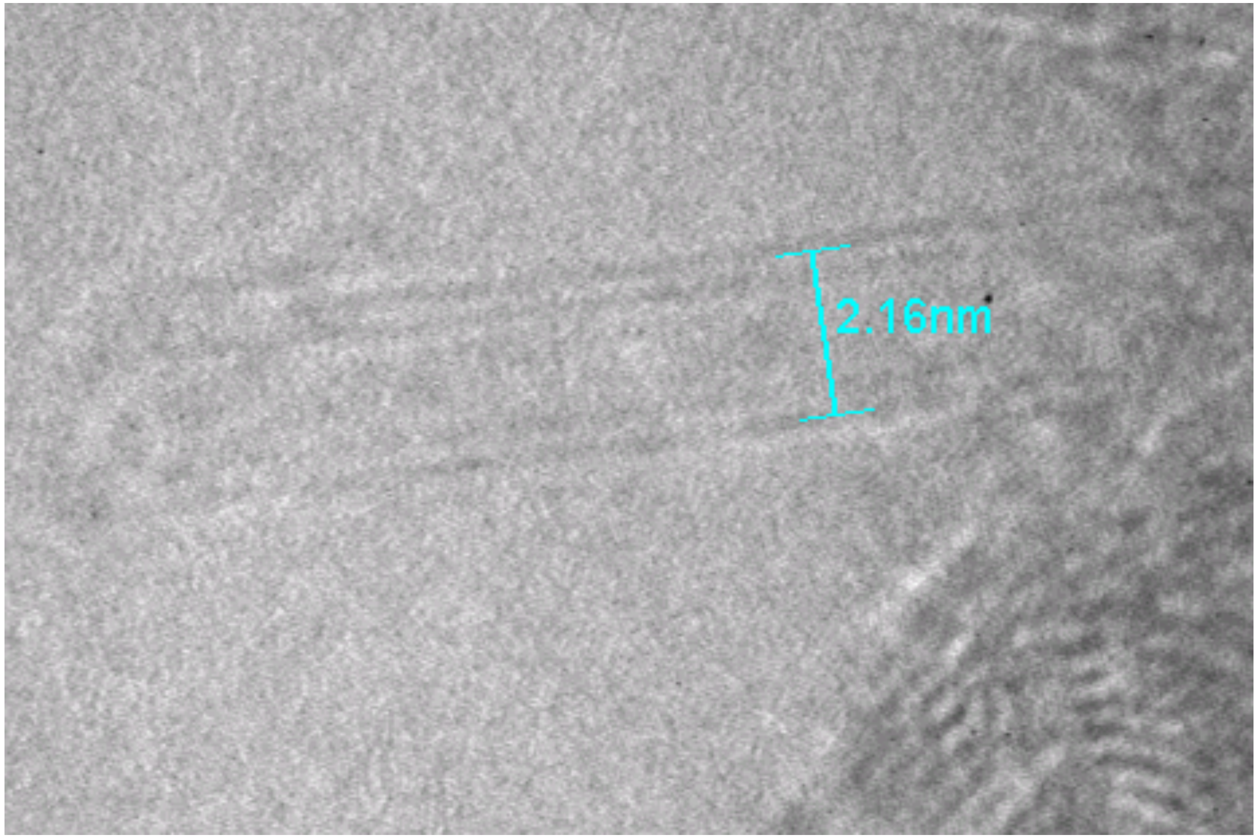
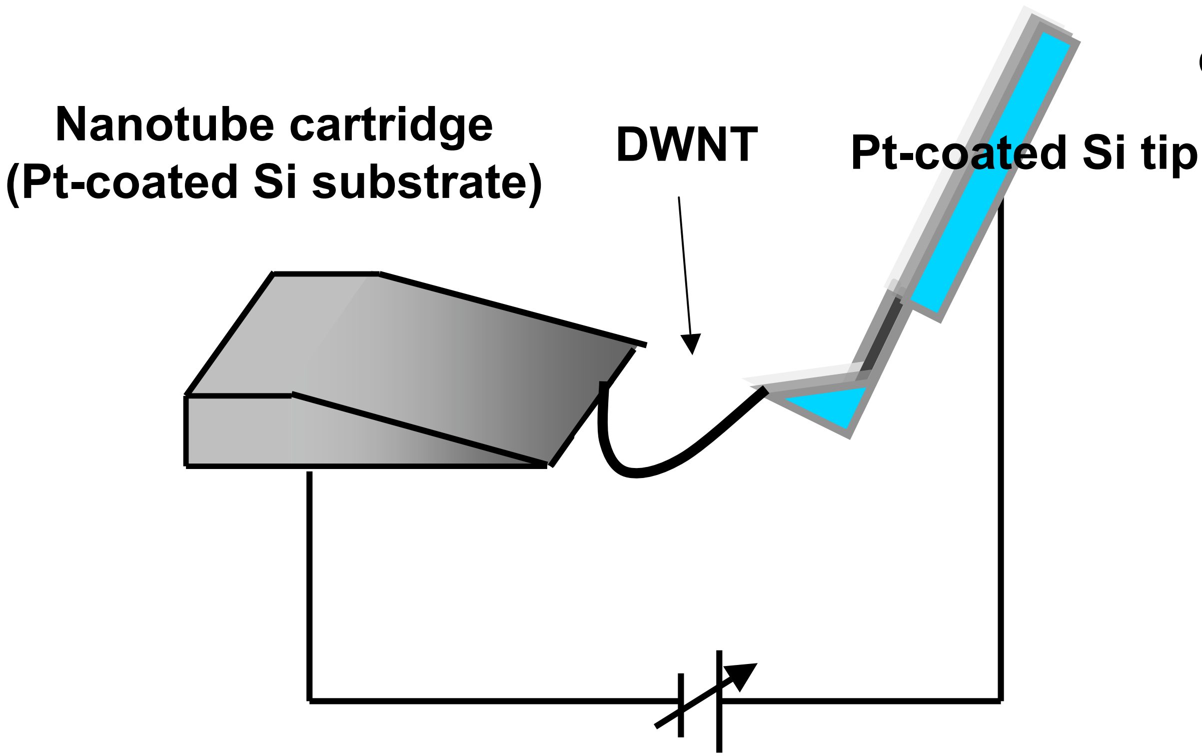
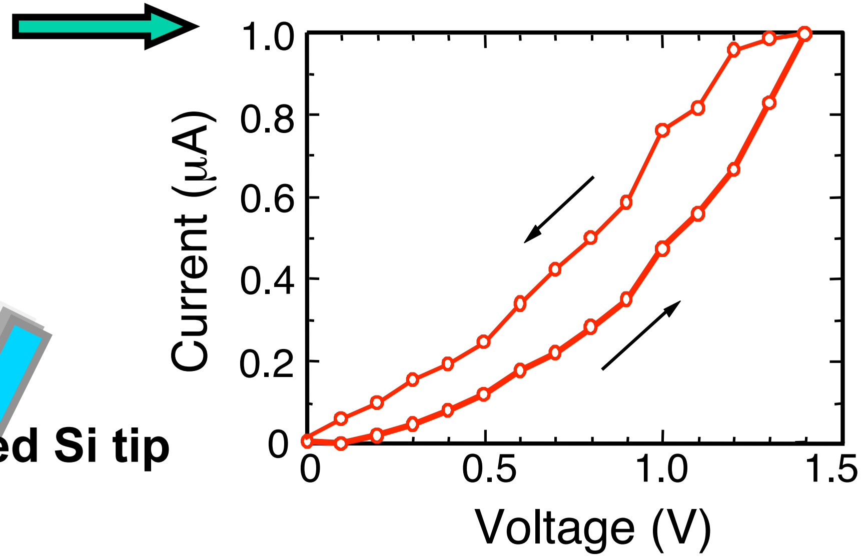
Typical DWNT used in this study



How to induce the plastic deformation





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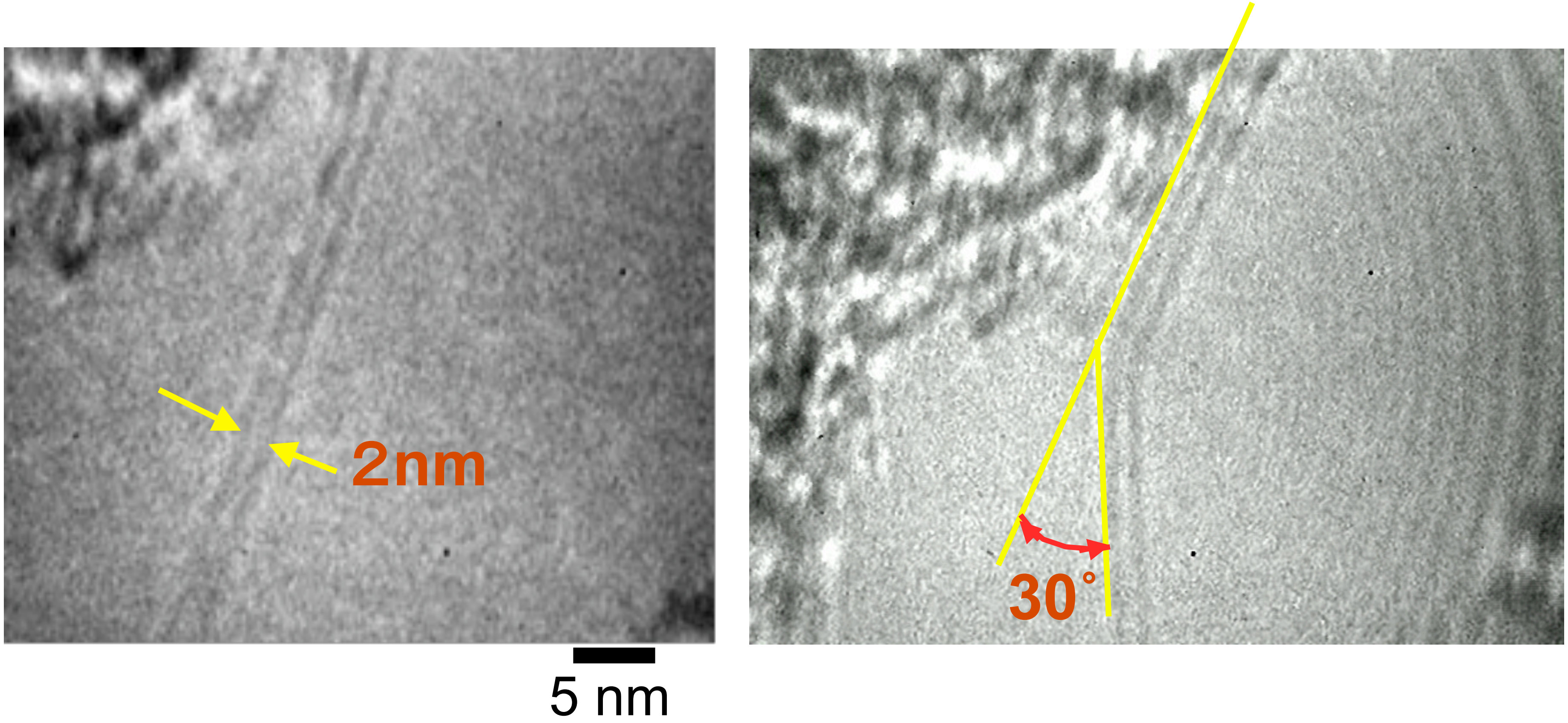
Current induced plastic deformation



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

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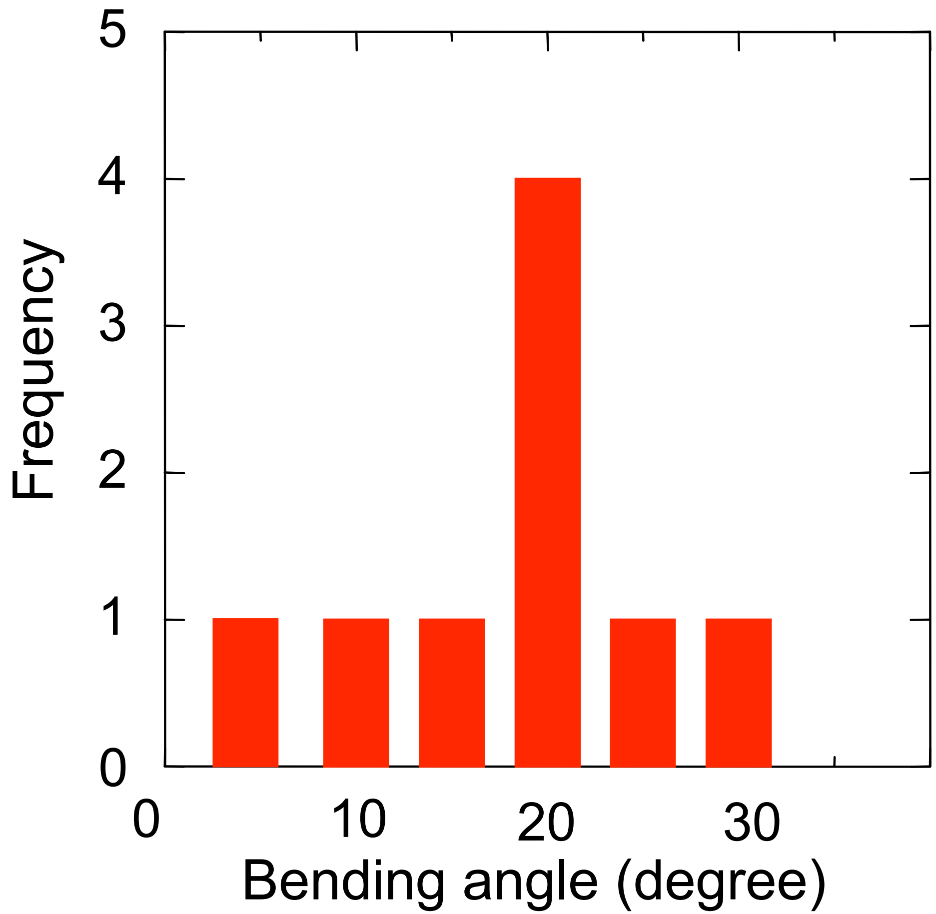
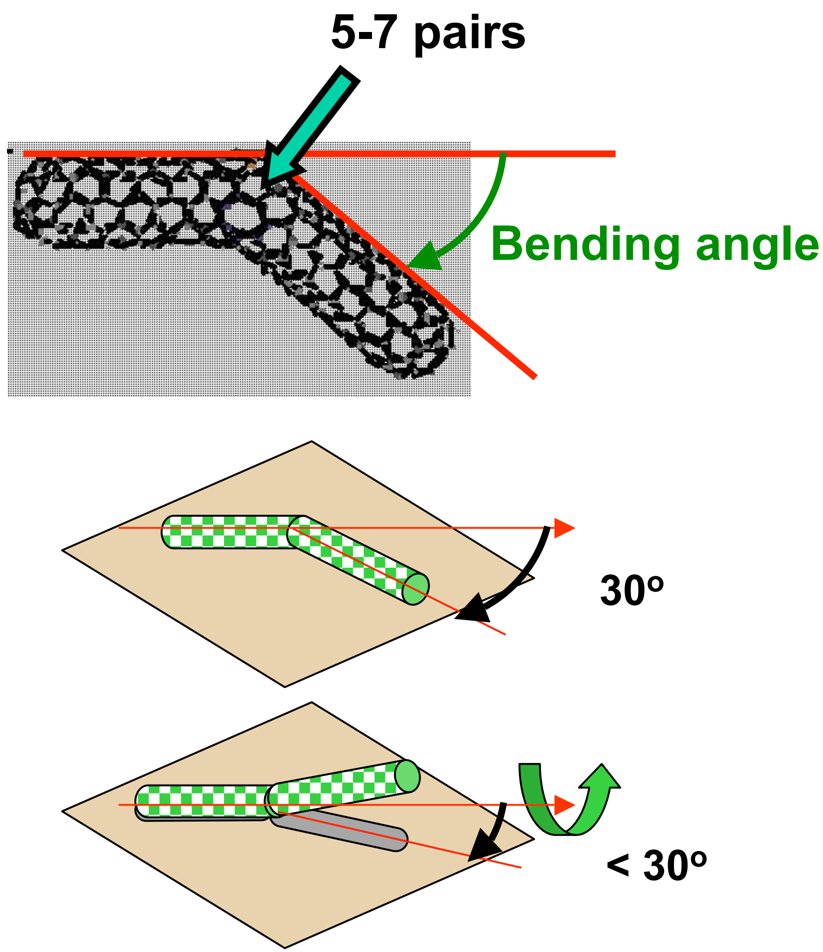
Bending angle of the plastic deformation





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

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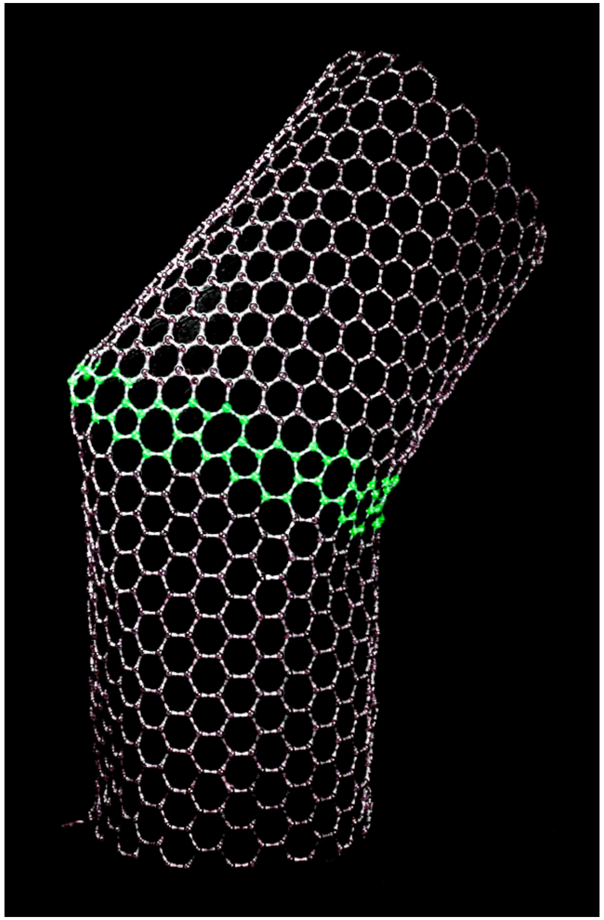
Model for (15,15) nanotube



(15,15) ; ϕ2nm

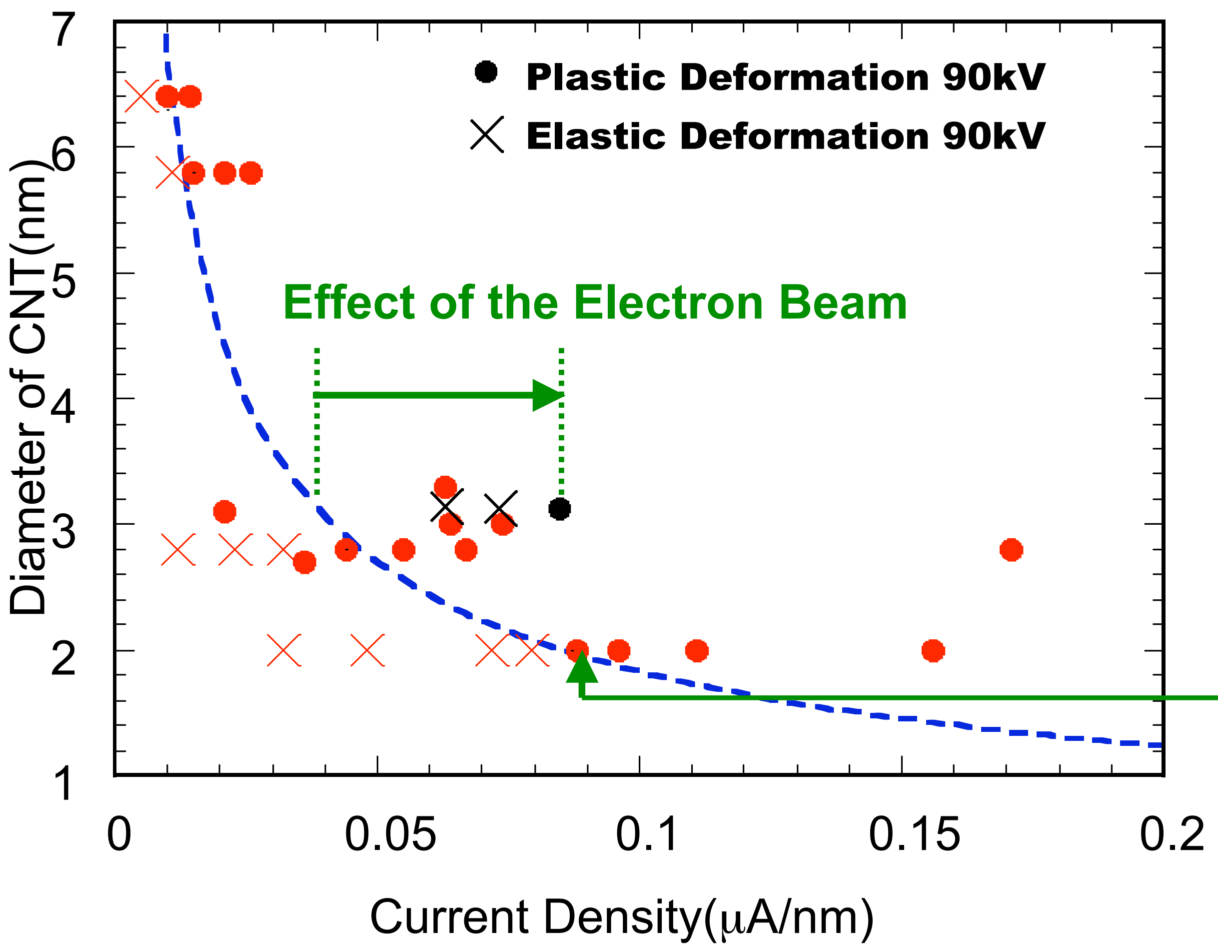
Nanotube consisting of balls and sticks

14 pairs of 5-7 rings

(with bending angle of 30°)

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

Dependence on diameter and electron beam



Sublimation

av. 2.2 μA/nm
(φ : 2nm)

Bend deformation

0.087μA/nm
(φ : 2nm)

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

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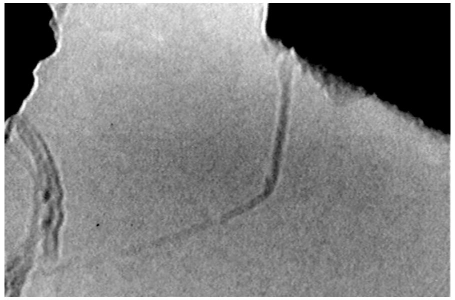
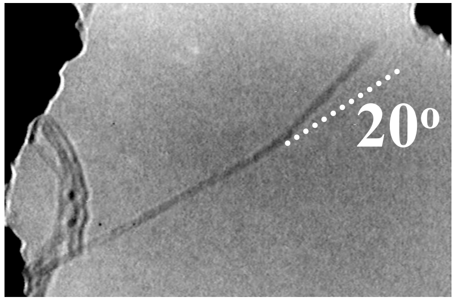
Recovery from bend deformation

Diameter of CNT : 3.3nm

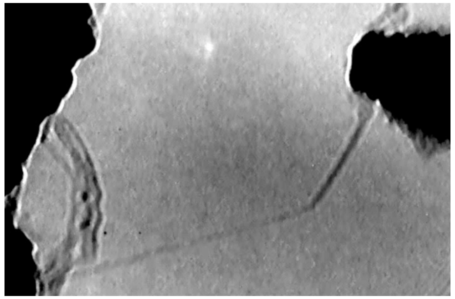
Original shape


Current under duress



Permanent bend

0.06μA/nm


Contact with the Si tip again

Applying more current to the bend portion

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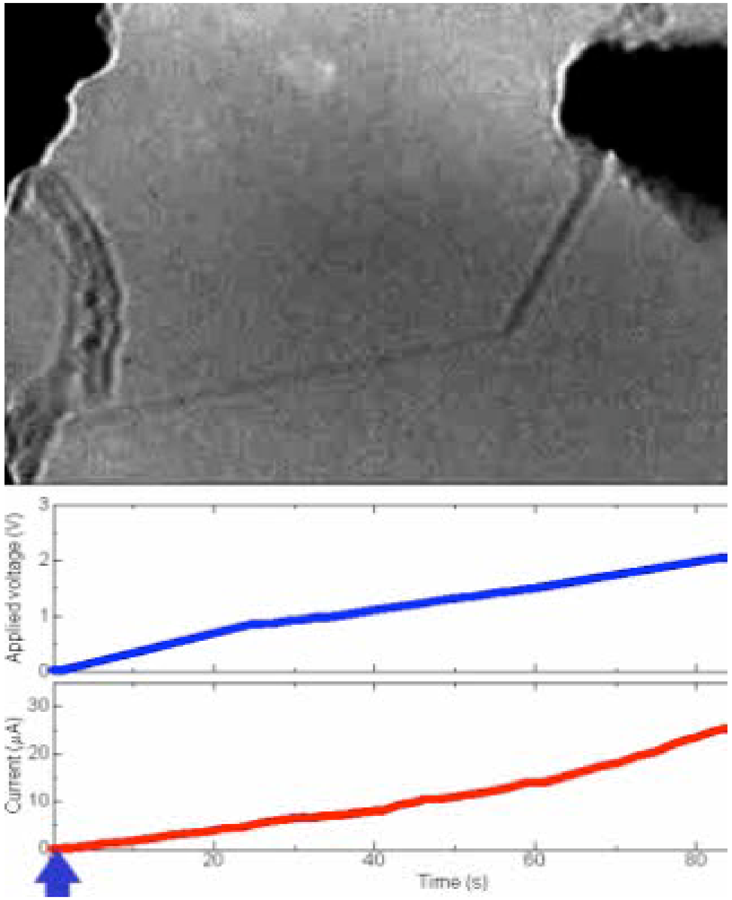
Demonstration of recovery from bend deformation

Diameter of CNT : 3.3nm

Voltage

Current



At 3.2 μA/nm the CNT becomes straight

3.2 μA/nm is comparable 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 results from the curing of defects of pentagon–heptagon pairs at∽2500K

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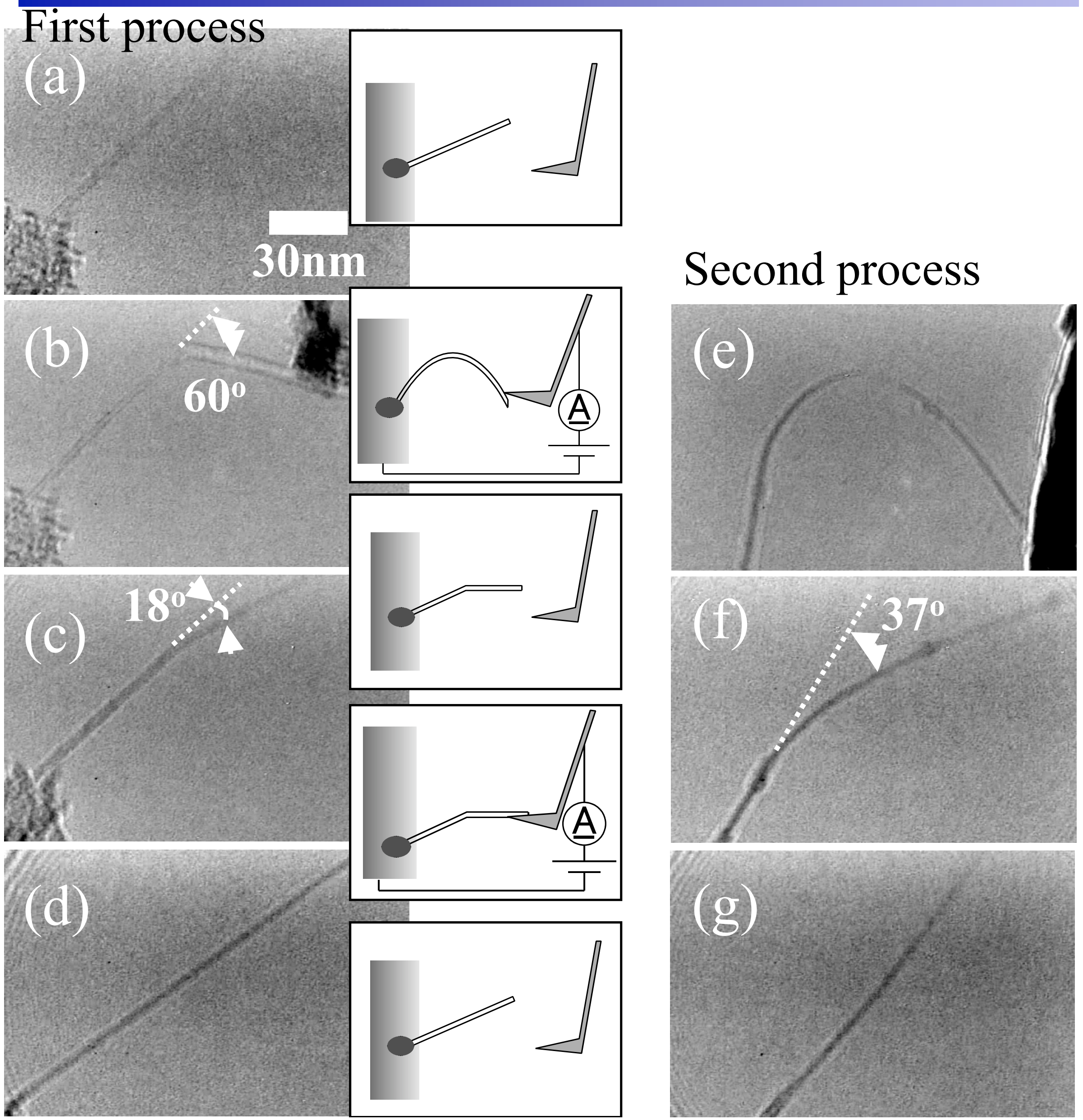
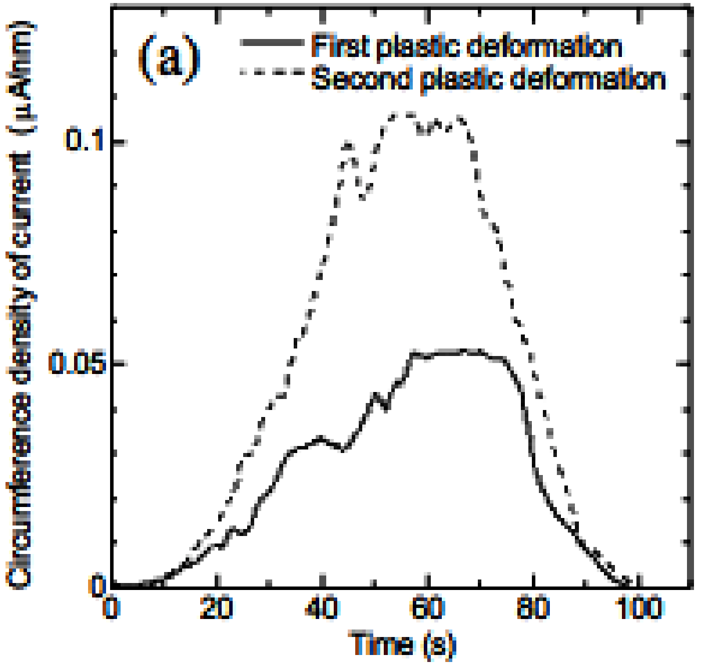
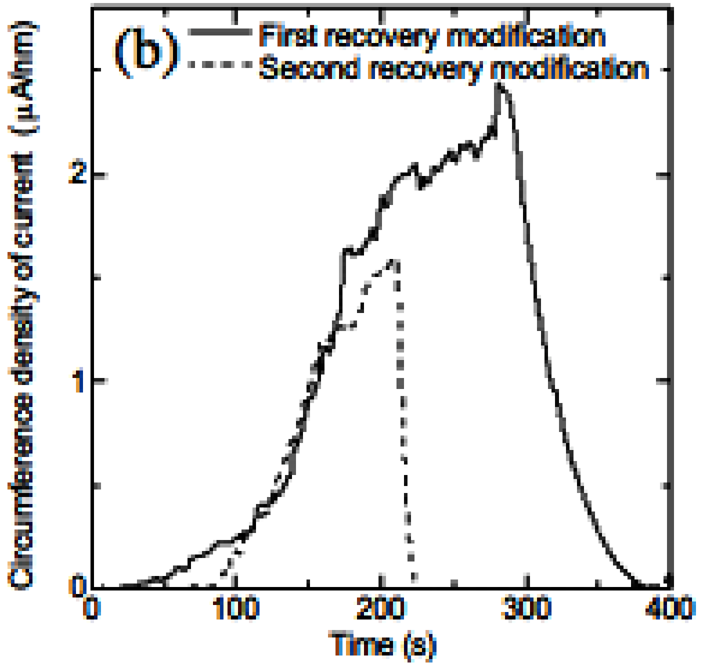
Reversible deformation

O. Suekane et. al., submitted

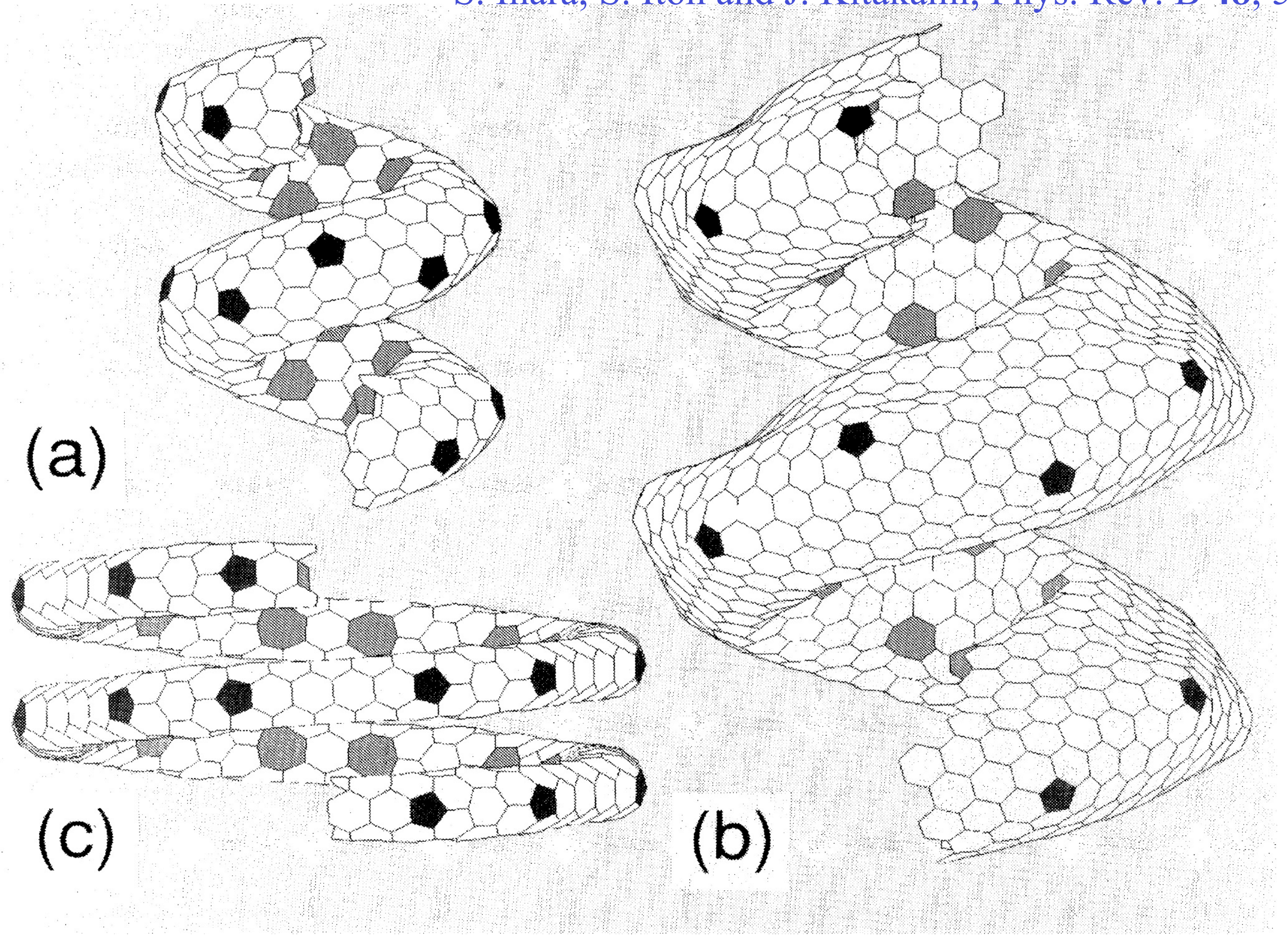






Confirmation of universality

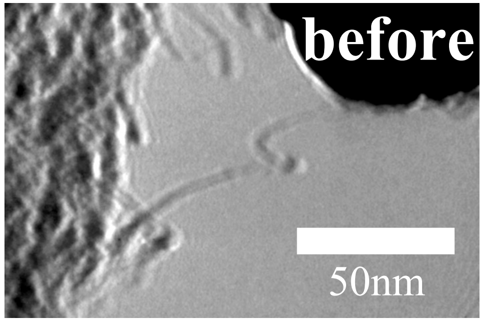
S. Ihara, S. Itoh and J. Kitakami, Phys. Rev. B **48**, 5643 (1993).

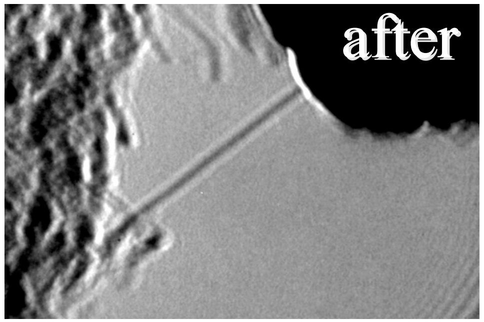


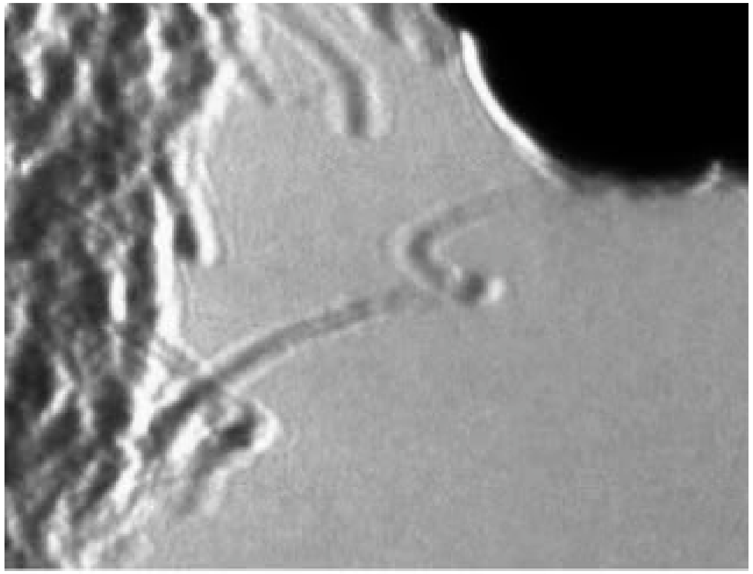
Coils have pentagons and heptagons, respectively,
in the outer and inner ridgelines. ⇒ Good example

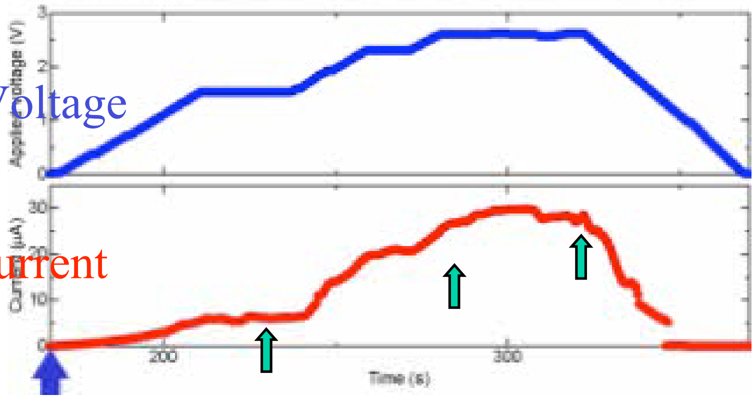
Demonstration of recover from helical

CNT diam.: 3.7nm
coil diam.: 18 nm

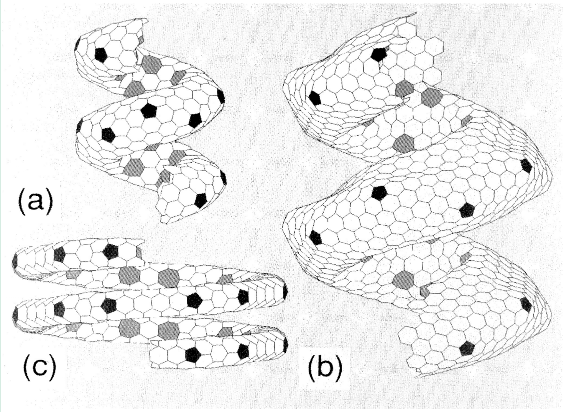








O. Suekane et. al., submitted



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 .

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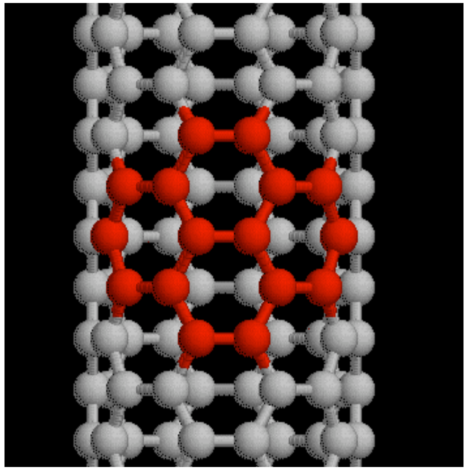
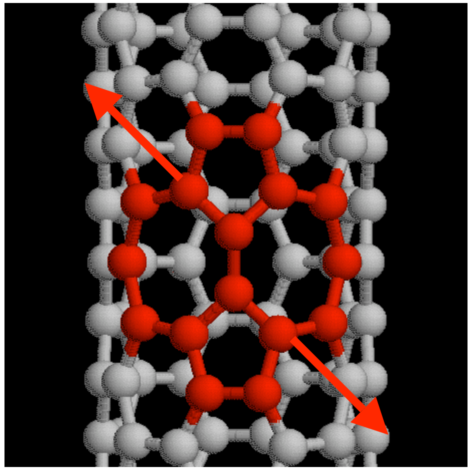
3 Summary

Analysis of energy pathways for forming plastic bend (1)

Visit poster D053

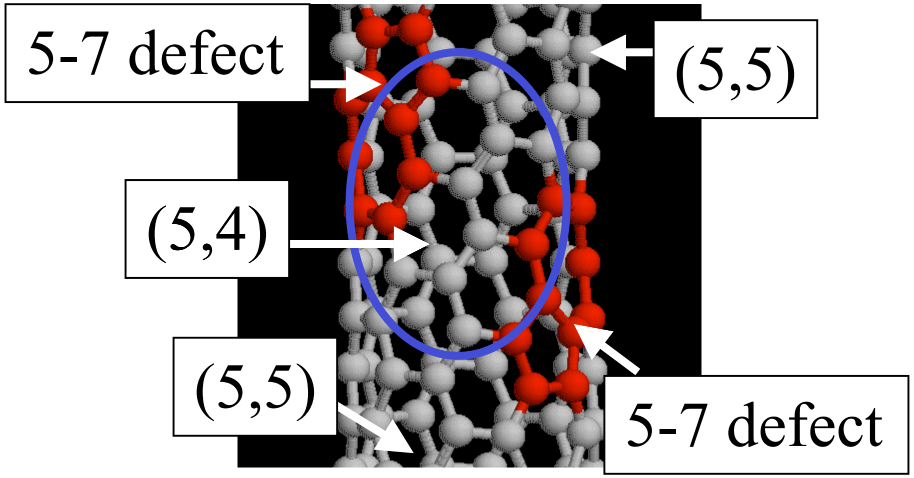
(5,5)





Assumption

1) keep sp^2 bond network
2) no square and no octagon
3) atoms: no generation
   no disappear



Nucleation of Stone-Wales defect

↓

Dissociation of Stone-Wales defect

↓

Splitting of 5-7 defects

↑

Energy pathways are studied using the nudged elastic band minimum energy path calculation.

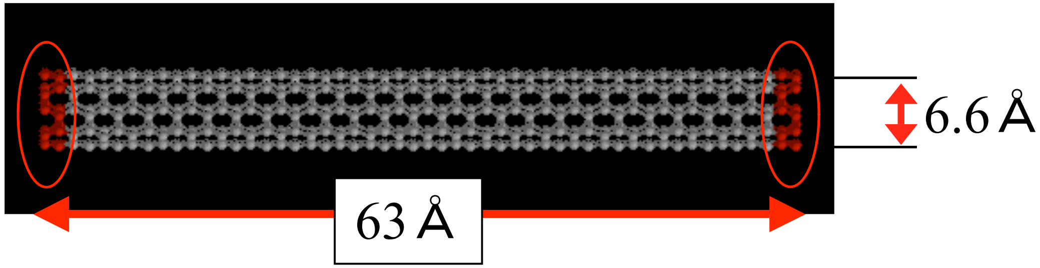
H. Mori et. al., submitted

Ref. B. I. Yakobson, APL, **72**, 918 (1998).

Analysis of energy pathways for forming plastic bend (2)

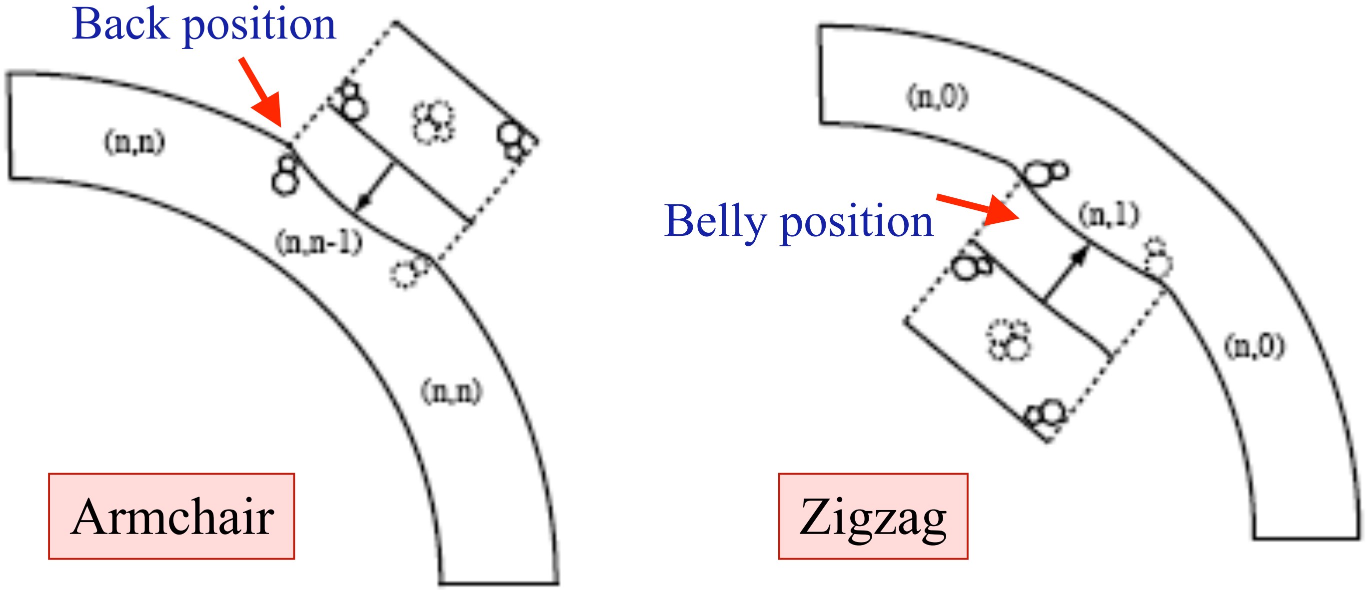
Visit poster D053

Two SWNTs:
(5,5) 63 Å 520 atoms
(8,0) 63 Å 480 atoms



Boundary condition:
- Ends are fixed.
- Others are free.

Potential:
Analytic bond-order potential of Pettifor and Oleinik)



H. Mori et. al., submitted

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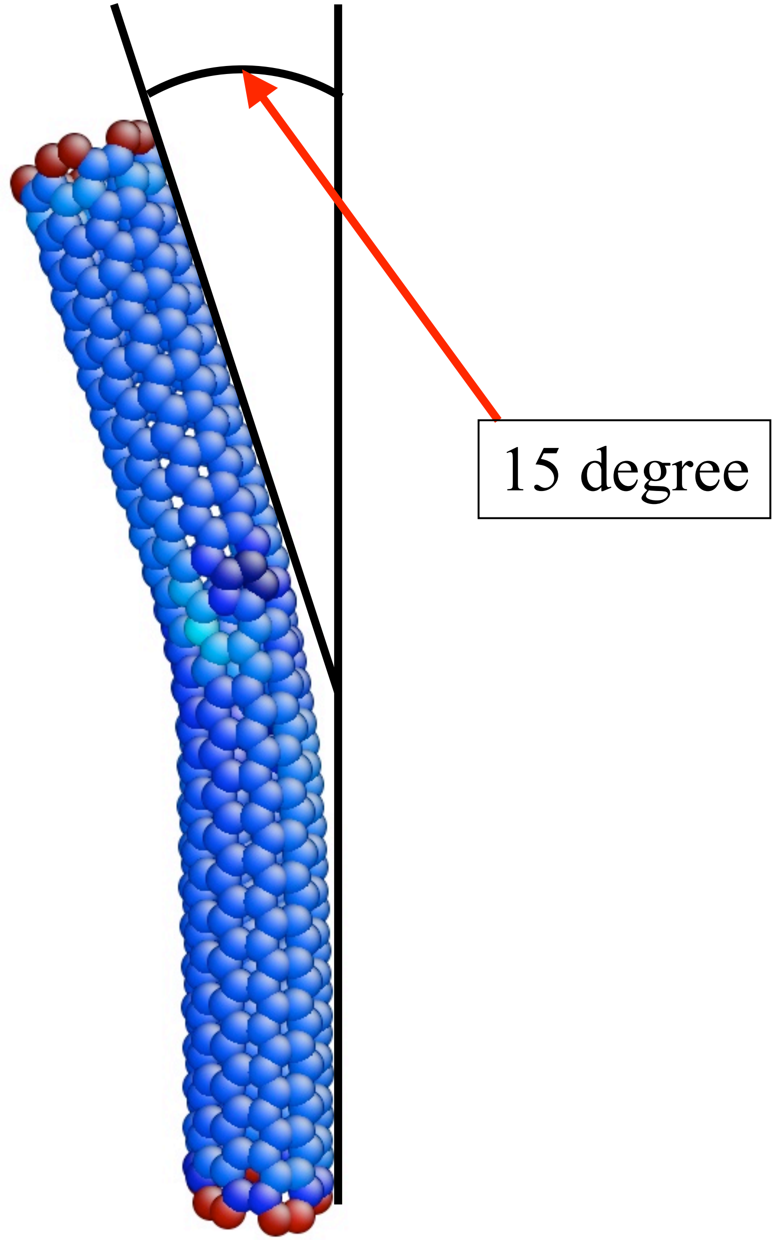
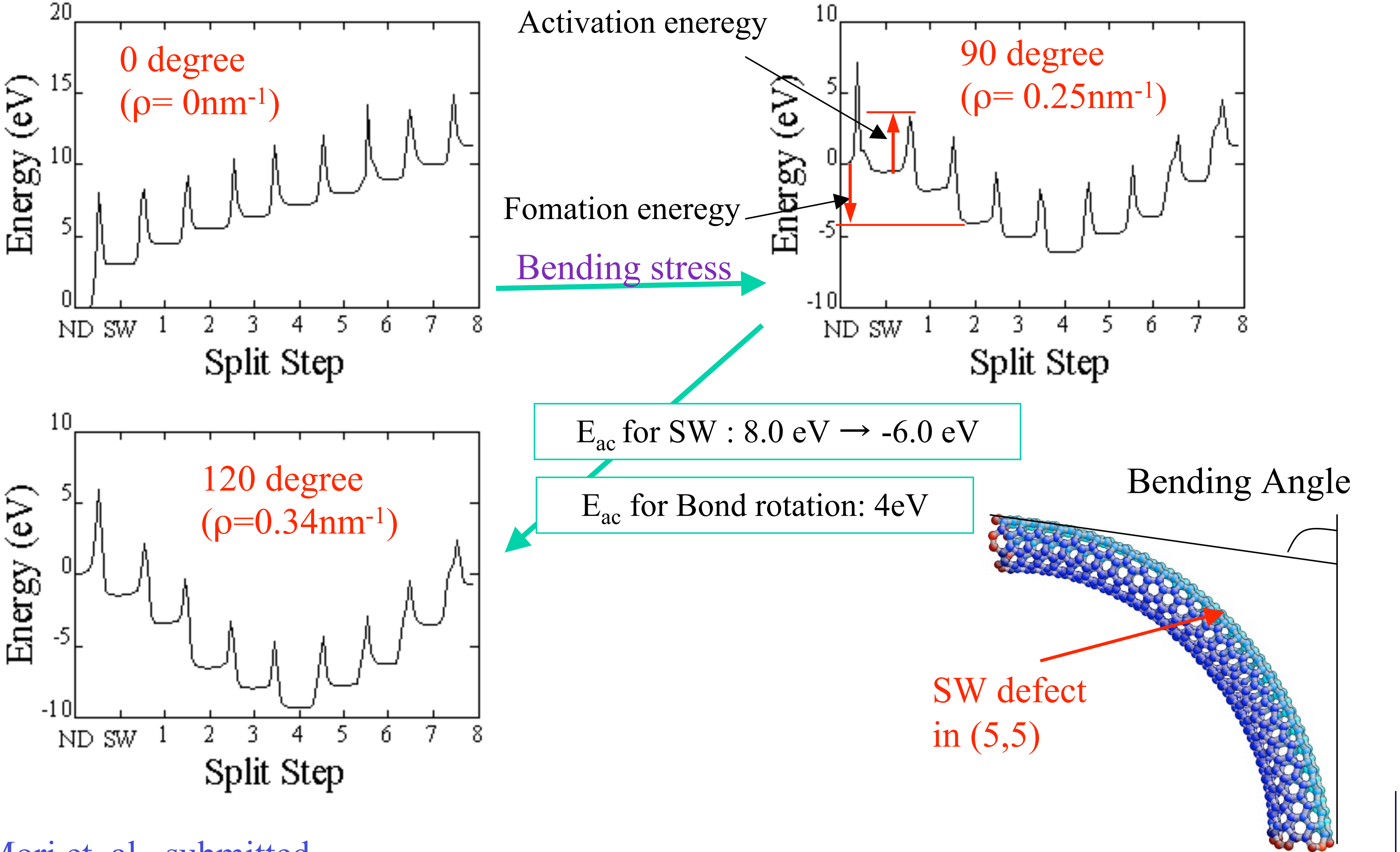
(5,5) Armchair SWNT



Minimum energy pathways in (5,5) SWNT



H. Mori et. al., submitted

Frequency of a bond rotation to form a S-W defect

Highest microscopic energy barrier in achieving plastic deformation is the activation barrier for Stone-Wales defect nucleation.

→ Arrenius equation

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

k_B :Boltzmann constant
$\nu = 10^{13}\ s^{-1}$
$T = 1500$K

$E_{act} = 4$ eV

↓

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

↓

One bond rotation occurs every few seconds at 1500K, consistent with experimental results.

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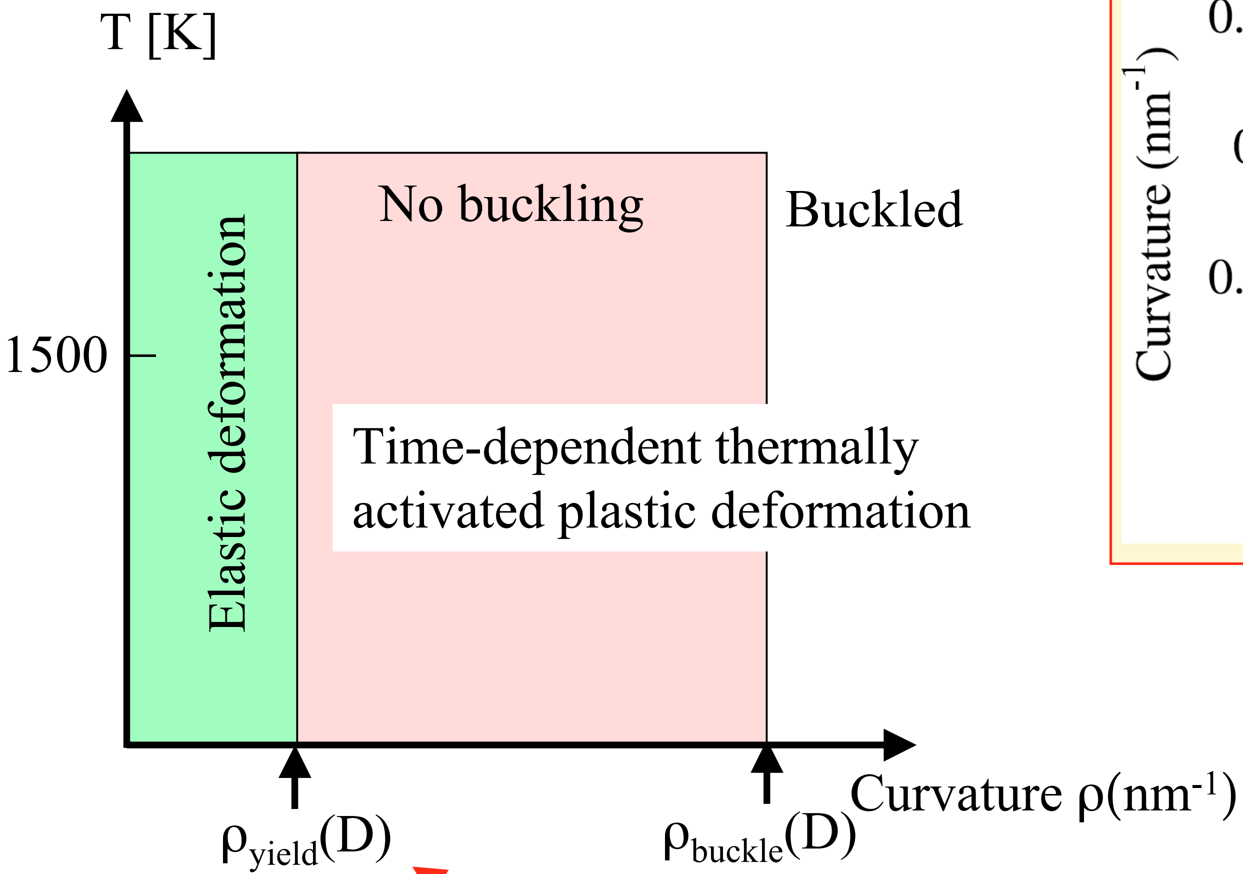
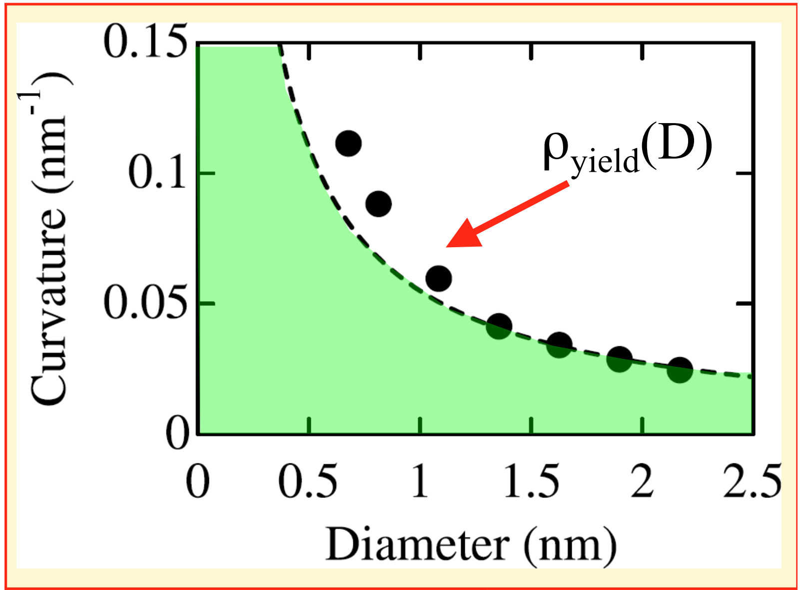
Deformation mechanism map for SWNT bending





Plastic deformation is time-dependent thermally activated when $\rho > \rho_{yield}$ depending on the chirality and diameter.

H. Mori et. al., submitted

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Summary

(1) The plastic bend deformation can be induced in a straight nanotube by the current flow less than 1/20 of that for the sublimation under the mechanical duress.

(2) The plastic bend is metastable and thus it can recover back to straight when the current density is comparable to the sublimation one.

(3) The theoretical analysis indicates that the yield curvature ρ_{yield} is defined and depends on diameter.

(4) Above ρ_{yield}, the plastic bend deformation is time-dependent thermally activated.

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