Current-Induced Reversible Deformation of Carbon Nanotubes

Y. Nakayama\textsuperscript{1,2)}
\textsuperscript{1)}Osaka Prefecture University
\textsuperscript{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)
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
      • Manipulation 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
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.

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.
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

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

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
Deposition time = 2 hr.

Visit poster A007
Development of high strength fibers, ropes, sheets using CNTs

Brush-type of CNTs

CNT yarn rolled up

Drawing and spinning a yarn (x200)
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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3 Summary
Super-nanofactory and CNT cartridge

Pt-coated Si-substrate

DWNT

Electron beam

CNT cartridge (Stage A)

Cantilever (Piezo-stage B)

GND (TEM Holder)
Typical DWNT used in this study
How to induce the plastic deformation

Nanotube cartridge (Pt-coated Si substrate)

DWNT

Pt-coated Si tip

Voltage (V)

Current (µA)

0
0.2
0.4
0.6
0.8
1.0

0
0.5
1.0
1.5

Osaka Prefecture University

frc
Current induced plastic deformation

Y. Nakayama et al., Jpn J. Appl. Phys. 44 L720.(2005)
Bending angle of the plastic deformation

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

Effect of the Electron Beam

Plastic Deformation 90kV
× Elastic Deformation 90kV

Sublimation
av. 2.2 µA/nm
(φ : 2nm)

Bend deformation
0.087 µA/nm
(φ : 2nm)

Y. Nakayama et al., Jpn J. Appl. Phys. 44 L720.(2005)
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3 Summary
Recovery from bend deformation

Diameter of CNT : 3.3nm

Original shape
Current under duress
Permanent bend

Applying more current to the bend portion

Contact with the Si tip again

$0.06 \mu A/nm$
Demonstration of recovery from bend deformation

Diameter of CNT : 3.3nm

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


This recovery results from the curing of defects of pentagon–heptagon pairs at ≈ 2500K
Reversible deformation

O. Suekane et. al., submitted
Confirmation of universality


Coils have pentagons and heptagons, respectively, in the outer and inner ridgelines. ➞ Good example
The coil started to loosen at $0.9 \, \mu\text{A/nm}$, drastically changed its structure at $2.2 \, \mu\text{A/nm}$.


O. Suekane et. al., submitted
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3 Summary
Analysis of energy pathways for forming plastic bend (1)  

(5,5)  

Assumption  
1) keep sp² 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  

Analysis of energy pathways for forming plastic bend (2)

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
(5,5) Armchair SWNT

15 degree
Minimum energy pathways in (5,5) SWNT

- 0 degree ($\rho = 0 \text{nm}^{-1}$)
- 90 degree ($\rho = 0.25 \text{nm}^{-1}$)
- 120 degree ($\rho = 0.34 \text{nm}^{-1}$)

Activation energy

Formation energy

Bending stress

$E_{ac}$ for SW : $8.0 \text{ eV} \rightarrow -6.0 \text{ eV}$

$E_{ac}$ for Bond rotation: $4 \text{ eV}$

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.

\[ f = \nu \exp\left(-\frac{E_{\text{act}}}{k_B T}\right) \]

\( E_{\text{act}} = 4 \text{ eV} \)

\( \nu = 10^{13} \text{ s}^{-1} \)

\( T = 1500 \text{K} \)

One bond rotation occurs every few seconds at 1500K, consistent with experimental results.
Plastic deformation is time-dependent thermally activated when $\rho > \rho_{\text{yield}}$ depending on the chirality and diameter.

H. Mori et. al., submitted
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3 Summary
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** $\rho_{\text{yield}}$ is defined and depends on diameter.

(4) Above $\rho_{\text{yield}}$, the plastic bend deformation is **time-dependent thermally activated**.