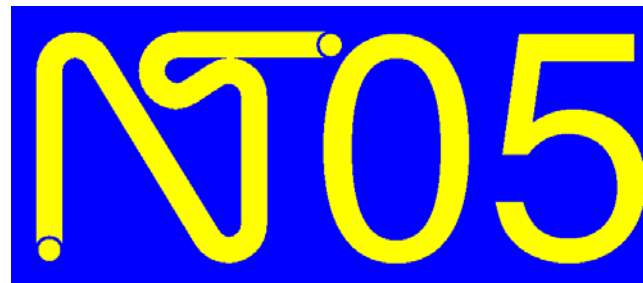


**NT05: Sixth International Conference on the  
Science and Application of Nanotubes**

***Göteborg, Sweden***

***June 26 - July 1, 2005***

**<http://nanotube.msu.edu/nt05/>**



## **Introduction to Focussed Poster Sessions, and Concluding Remarks at NT'05**

A.1	<b>Annick Loiseau</b>	Monday, June 27
A.2	<b>Esko I. Kauppinen</b>	Tuesday, June 28
A.3	<b>Marcos Pimenta</b>	Tuesday, June 28
A.4	<b>Jack Fischer</b>	Tuesday, June 28
B.1	<b>Pavel Nikolaev</b>	Thursday, June 30
B.2	<b>Apparao Rao</b>	Thursday, June 30
B.3	<b>Tony Heinz</b>	Thursday, June 30
B.4	<b>Gianaurelio Cuniberti</b>	Friday, July 1
B.5	<b>Yoshiyuki Miyamoto</b>	Friday, July 1
CR	<b>Mildred Dresselhaus</b>	Friday, July 1

## NT'05 SCIENTIFIC PROGRAM

Time	Sun 26	Mon 27	Tues 28	Wed 29	Thurs 30	Fri 1		
08:30-09:00		registration	registration					
09:00-09:45			Maurizio Prato	Morinobu Endo	David Tomanek	Paul L. McEuen		
09:45-10:15		Welcoming address (09:30-10)	Alan Windle	Susumu Katagiri	Jean-Louis Sauvajol	Nadine Kam		
10:15-10:45		Sumio Iijima (10-10:45)	Jerry Tersoff	Jean Dijon	Junichiro Kono	Cheol Jin Lee		
10:45-11:15		Steven G. Louie	Coffee	Coffee	Coffee	Coffee		
11:15-11:45		Coffee	Young Hee Lee	Jong-Min Kim	Tony Heinz	Brian LeRoy		
11:45-12:05		Humberto Terrones (11.45-12.15)	Yoshinori Sato	Atsuko Nagataki	A.V. Krashennikov	S. W. Lee		
12:05-12:25		Lars Samuelson (12.15-12.45)	lunch	A. K. Swan	lunch	lunch		
12:25-14:00		lunch (12.45-14.20)		lunch				
14:00-14:20			Pavel Nikolaev	Boat trip and conference dinner	G. Seifert	Perti Hakonen		
14:20-14:40		Feng Ding	Vincent Jourdain		B. Gao	A. Wall		
14:40-16:00		Masahiko Ishida (14.40-15)					Poster Session B	
16:00-18:00	registration	Poster Session A	Poster Session A	conference dinner	Poster Session B			
18:00-19:00	Welcome party							Snacks 19:00
19:00-21:00		Göteborg reception						Concluding Remarks 20.00

Welcoming address at 09:30 on Monday by the Chancellor of Göteborg University.

Welcome party, welcoming address, registration, talks, posters, lunch and Friday evening snacks are in the Chalmers University Student Union Building, located at the main entrance to Chalmers University of Technology.

Göteborg Reception is on Monday evening at 'Börsen' in the heart of Göteborg, about 30 minutes walk from the Student Union. Guides (if needed) leave the Student Union at 18:15.

On Wednesday buses leave from the Student Union to the boat trip at 14:00.

Poster sessions include reports by the poster chairs

## Posters

Poster abstracts are listed from page XX, and are identified according to a sorting category given below.

Posters in categories I-VIII will be presented in Session A (Monday and Tuesday).

Posters in categories IX-XXI will be presented in Session B (Thursday and Friday).

- I. CVD Synthesis of Carbon Nanotubes
- II. Non-CVD Synthesis of Nanotubes
- III. Formation and Characterization of Unusual Nanostructures
- IV. Raman Characterization of Nanotubes
- V. Other Characterization of Nanotubes
- VI. Nanotube Dispersion and Purification
- VII. Chemical Modification of Nanotubes
- VIII. Non-Carbon Nanotubes
- IX. Nanotube-Based Composites
- X. Morphology and Application of Modified Nanotubes
- XI. Photo-Induced Reactions in Nanotubes
- XII. Thermal and Mechanical Properties of Nanotubes
- XIII. Atomic Structure of Carbon Nanotubes
- XIV. Transport in Nanotubes
- XV. Field Electron Emission
- XVI. Optical Properties and Optoelectronics
- XVII. Transport in Complex Nanostructures
- XVIII. Electron-Phonon Coupling in Complex Nanostructures
- XIX. Nanotube-Based Transistors
- XX. Magneto-Transport and Magnetism
- XXI. General Studies of Carbon Nanostructures

## NT'05 contributions

In the spirit of the NT Conference series, oral presentations will consist of plenary, keynote and contributed talks. However, most contributions are presented as posters, and over half of the conference is dedicated to the poster exhibitions. Due to the large number of poster presentations, the NT'05 program does not include the two minute 'poster+' presentations that were a feature of preceding NT conferences. Instead, posters will be introduced by poster 'chairs', which leaves most of the time for discussion at the individual posters.

There are two poster sessions.

- Session A is on Monday and Tuesday and includes posters I.1 – VIII.12.
- Session B is on Thursday and Friday and includes posters IX.1 – XXI.30

These two sessions are divided into sub-sessions that will be introduced by the chairs. In addition, it is expected that contributors are available at their posters after the presentation of their sub-session.

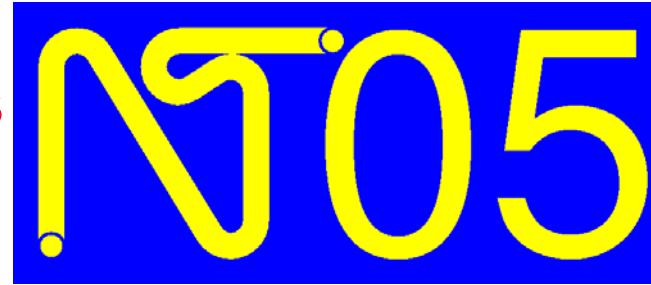
<b>Sub-session</b>	<b>Posters</b>	<b>Poster chair</b>	<b>Presentation by chair</b>
A.1	I.1-I.40	Annick Loiseau	Monday, June 27
A.2	I.41-I.81	Esko I. Kauppinen	Tuesday, June 28
A.3	II-IV	Marcos Pimenta	Tuesday, June 28
A.4	V-VIII	Jack Fischer	Tuesday, June 28
B.1	IX-X	Pavel Nikolaev	Thursday, June 30
B.2	XI-XIII	Apparao Rao	Thursday, June 30
B.3	XIV	Tony Heinz	Thursday, June 30
B.4	XV-XVIII	Gianaurelio Cuniberti	Friday, July 1
B.5	XIX-XXI	Yoshiyuki Miyamoto	Friday, July 1

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**A.1 Annick Loiseau**

**Monday, June 27**

POSTER SESSION A I1 - I40

Syntheses via CV techniques

# A few words about CVD

- Principle:*
- Decomposition of a carbonaceous gas at the surface of a metallic particle in a furnace ( $T = 500 - 1100^{\circ}\text{C}$ )
  - metallic particles prepared on a substrate prior to reaction with C gas or in situ

CVD are more and more used for the synthesis of MWNTs and SWNTs due to many advantages:

- flexibility: choice of the substrate, possible localized growth
- control of the catalyst preparation and particle size
- control of NT diameter and possibly helicity
- possible oriented growth (alignment)
- the most promising route to high purity samples with no need of costly post synthesis purification processes
- the most promising technique for industrial production
- synthesis of selectively MWNT, DWNT and SWNT
- heteroatomic tubes, doping, filling...

# Highlights of the session - 1

- Majority of studies concern synthesis of SWNT

22 : SWNT (I5, 6, 9, 10, 11, 12, 17, 19, 21, 23, 24, 25, 26, 29, 30, 34-40)

16 : MWNT (I2, 3, 4, 7, 8, 14, 15, 16, 18, 20, 22, 27, 28, 32, 33, 38)

1: DWNT (I13)

- Nature of the CVD process used:

PECVD : now for both MWNT (I2, I3, I18) and SWNT (I21, 25, 26, 35)  
(discussion of interest of PECVD for SWNT in I26, 35)

thermal CVD (I19, 29, 38)

Fluidized bed (I7, 34, I37)

Aerosol (I10, 15, 39)

Hot filament (I27, 40)

New techniques: continuous injection of prepared supported Fe (I6)

Hot wire generator (I11, 12)

laser irradiated CVD (I24)



# Highlights of the session -2

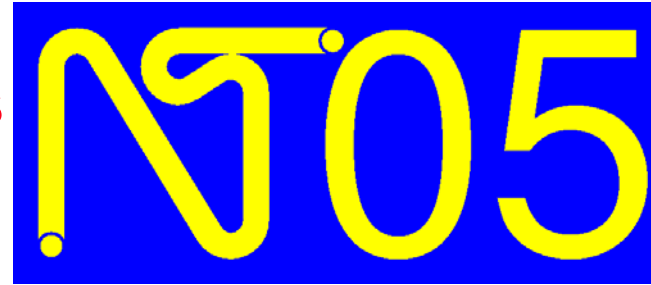
- Studies on the catalyst: preparation nature  
12 posters (I2, 9, 10, 11, 19, 20, 23, 28, 33, 36, 38, 40)
- Studies on the growth conditions , growth mechanism:  
7 posters (I7, 12, 15, 18, 29, 30, 34, 37)  
special mention to synthesis on membranes allowing direct  
TEM observations (I12, 17)
- Modeling of growth:  
3 posters (I1, 5, 31) but see also other sessions !
- Growth of NT in devices:  
2 posters ( I8, 17)
- Filling MWNT:  
3 posters (I14, 22, 27)
- Alignement:  
2 posters (I15, 25)

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**A.2 Esko I. Kauppinen**

**Tuesday, June 28**

**HIGHLIGHTS IN POSTER SESSION A.2.**

**POSTERS I.41 – I.81**

**CVD SYNTHESIS**

**Tuesday June 28 14:45 – 16:30**

**by**

**Esko I. Kauppinen**

**Dept. of Physics & Center for New Materials,**

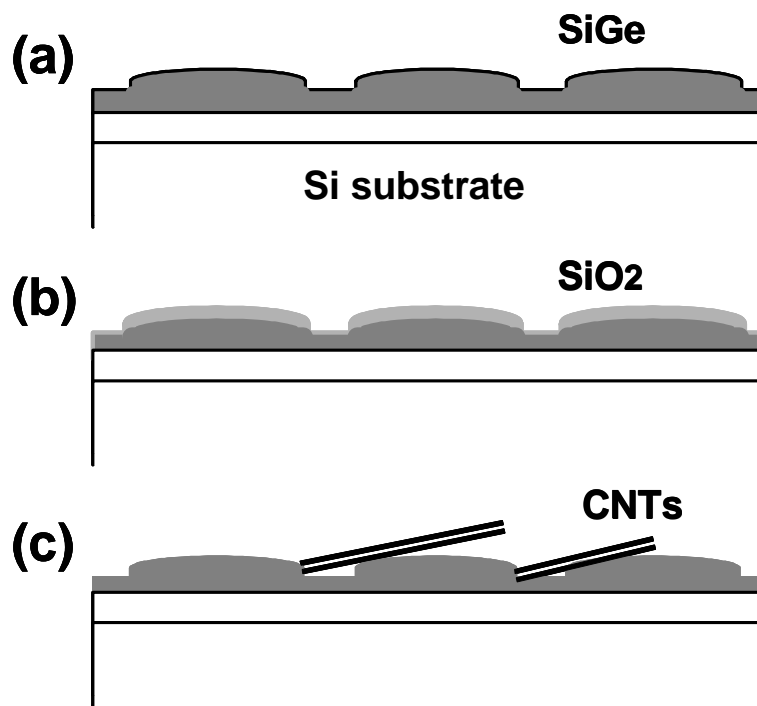
**Helsinki University of Technology (HUT)**

## Novel Approaches

- \* **Catalyst free CVD growth of SWCNT – I46**
- \* **Nano-contact printing of colloidal catalyst nanoparticles – I59**
- \* **Three-dimensional internal order of N-doped MWCNT – I60**
- \* **Aligned growth of SWCNT utilizing the crystalline structure of oxide catalyst support - I67**
- \* **Use of carbon-13 isotope to study precursor reaction mechanisms during ACCVD of SWCNT – I69**

# Metal catalyst free low temperature direct growth of carbon nanotubes on SiGe islands and Ge quantum dots

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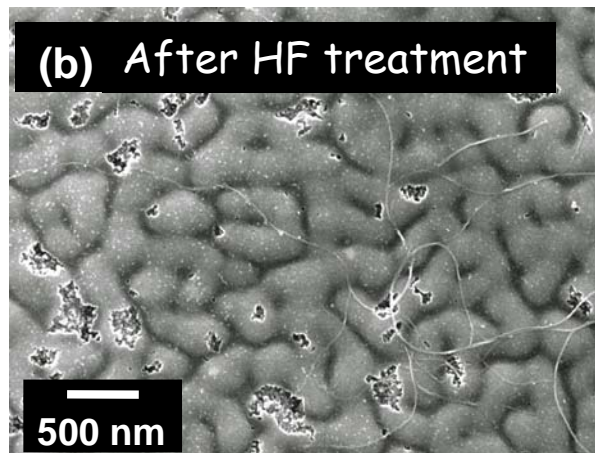
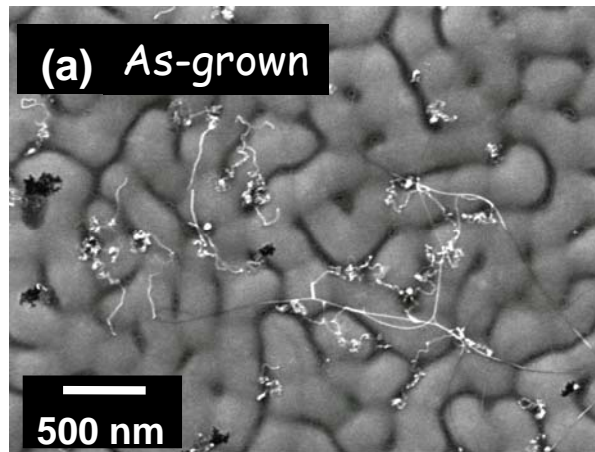


- 50 nm thick SiGe (Ge 30%) islands were grown on the Si substrates by CVD.
- C ion implantation: 2%
- Formation of 0.5 nm oxide by chemical oxidation with H<sub>2</sub>O<sub>2</sub>.
- CNT growth by CVD using CH<sub>4</sub> (1slm) and H<sub>2</sub> (0.3slm) at 850°C after preheating at 1000°C.

Fig.1. Schematic diagram process flow of CNT growth.

# Metal catalyst free low temperature direct growth of carbon nanotubes on SiGe islands and Ge quantum dots

---



- Two types of fibers were observed  
Thick, curly oxide fibers  
Thin, straight carbon nanotubes
- Oxide fibers were removed by HF
- Carbon nanotubes were removed by annealing in air above 400 °C
- EDX measurements detected no metal contaminants

Fig.2. SEM images of the fabricated nanofibers

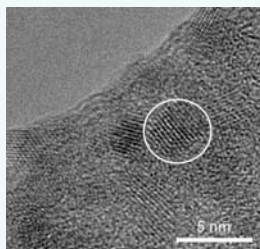
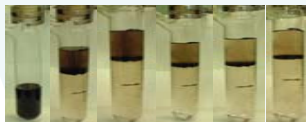
# NANO-CONTACT PRINTING OF COBALT COLLOID CATALYST FOR GROWTH OF VERTICALLY ALIGNED CARBON NANOTUBES

M. Cantoro<sup>1</sup>, V. B. Golovko<sup>2</sup>, S. Hofmann<sup>1</sup>, H. W. Li<sup>2,3</sup>, B. Kleinsorge<sup>1</sup>, J. Geng<sup>2</sup>, Z. Yang<sup>2,3</sup>, D. A. Jefferson<sup>2</sup>, A. C. Ferrari<sup>1</sup>, B. F. G. Johnson<sup>2</sup>, W. T. S. Huck<sup>2,3</sup>, J. Robertson<sup>1</sup>

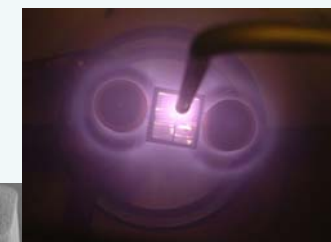
1 Engineering Dept.  
2 Chemistry Dept.  
3 Nanoscience Centre

Chemistry, nanofabrication, and carbon nanotube growth techniques are brought together to realize uniform arrays of vertically aligned CNTs by nano-contact printing.

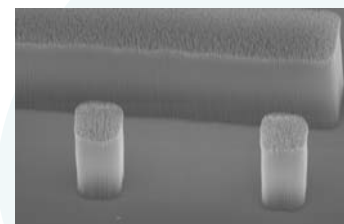
## CHEMISTRY



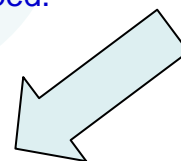
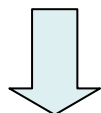
A highly purified and concentrated Co colloid to act as a catalyst for CNT growth has been developed. Co nanoparticles are 2-4 nm in diameter.



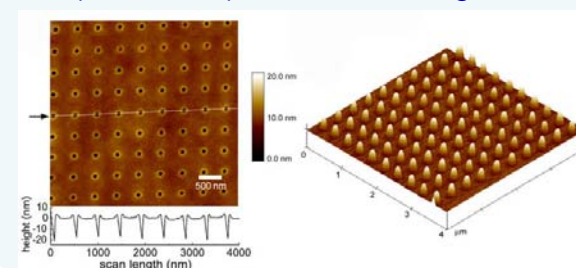
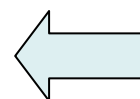
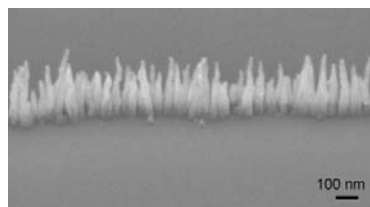
## CNT GROWTH



Plasma-Enhanced CVD conditions has been optimised to grow well-defined vertically aligned carbon nanotubes.



A nano-contact printing stamp to enable catalyst ink to be printed in nano-sized patterns (dots, lines), has been designed.



## NANOFABRICATION

After CNT growth, patterns are uniform over large areas. Nano-contact printing provides feature sizes down to **100 nm**, small enough to allow the nucleation of single, isolated and small diameter CNTs.

Nano-contact printing is a **low-cost, large-area, reliable** patterning method, alternative to e-beam lithography and other patterning techniques.

# Aligned Growth of Isolated Single-Walled Carbon Nanotubes Programmed by Atomic-Arrangement of Crystalline Surfaces

H. Ago,\* K. Nakamura, K. Ikeda, N. Uehara, and M. Tsuji

*Kyushu University, Fukuoka 816-8580, Japan*

- 1) SWNTs were aligned horizontally on R- and A- face sapphire substrates by CVD
- 2) The growth directions were associated with the crystalline orientations
- 3) Surface Al atoms are likely to guide the SWNT growth

SWNTs/sapphire (R-face  $\text{Al}_2\text{O}_3$ )

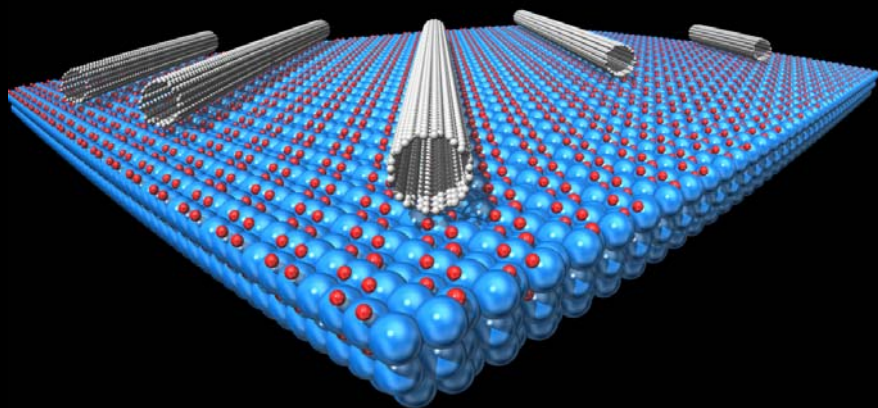
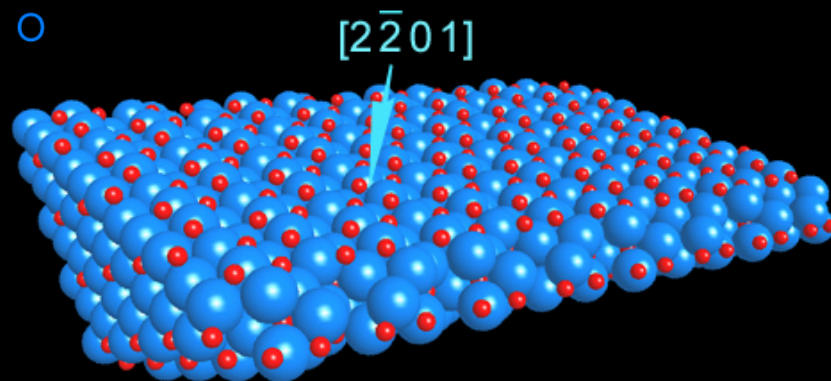
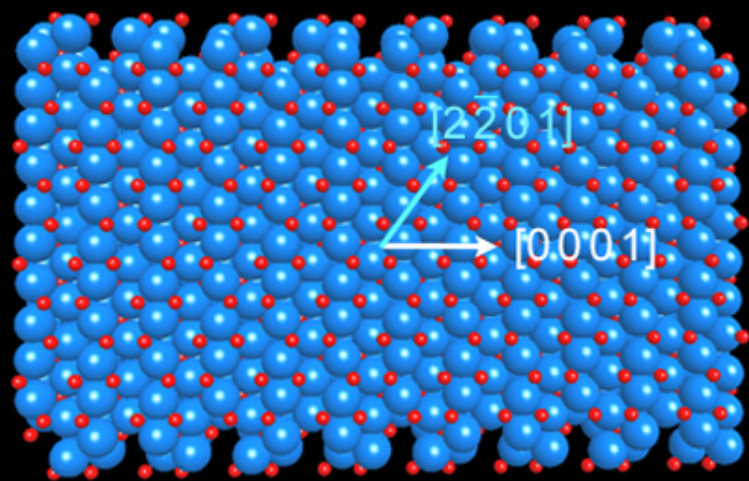
50  $\mu\text{m}$

SWNTs/sapphire (A-face  $\text{Al}_2\text{O}_3$ )

1  $\mu\text{m}$

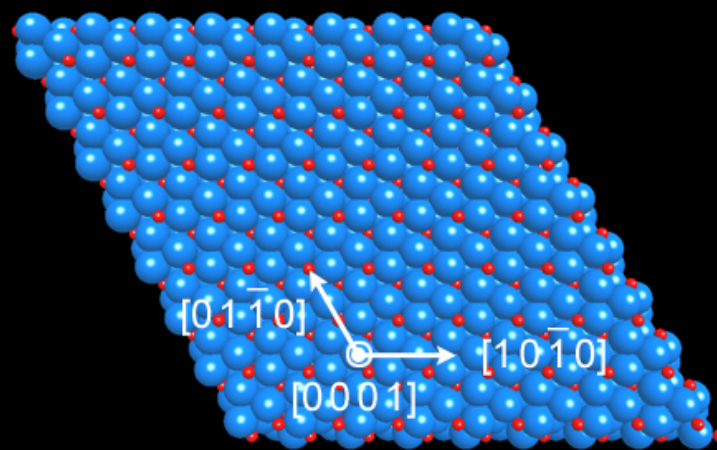


## A-face



Al atoms guide the SWNT alignment  
=> strong Al-SWNT attractive interaction

## C-face



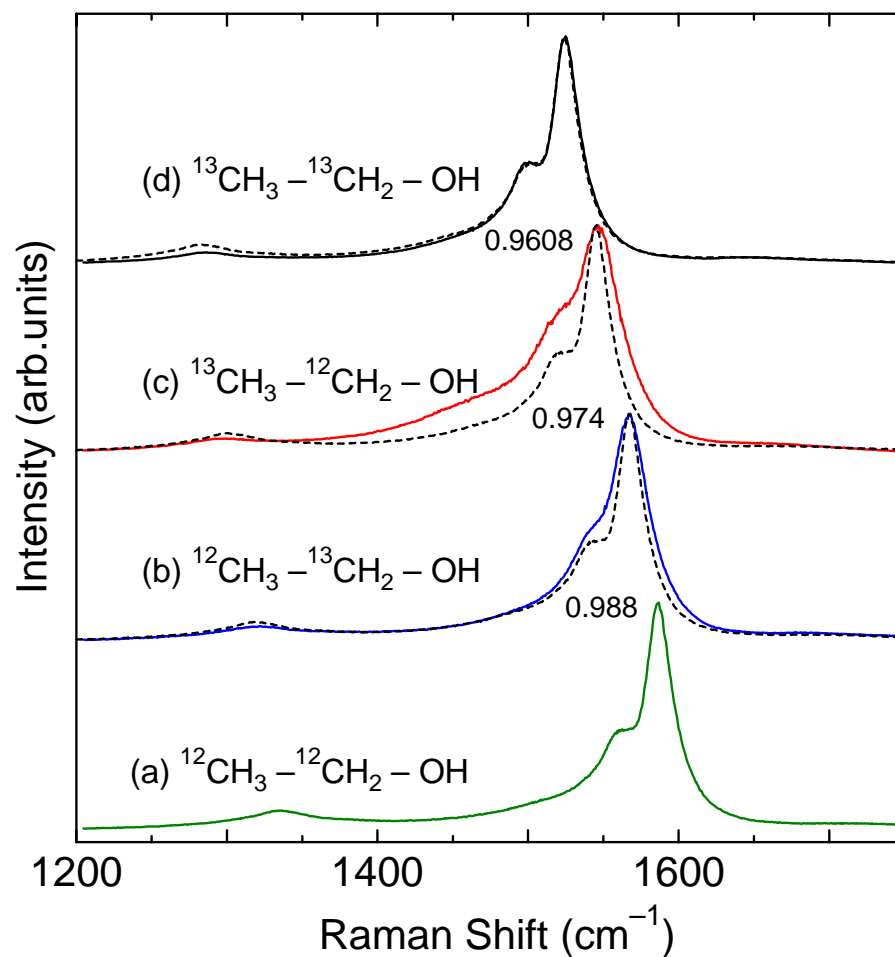
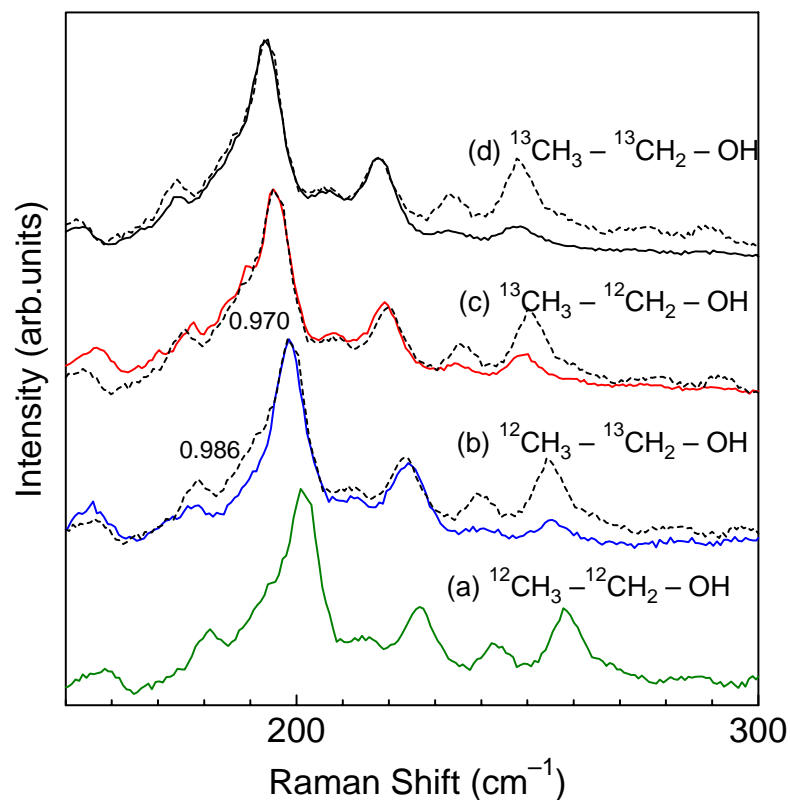
$C_3$  symmetry => No SWNT alignment

# Alcohol CVD Growth, Raman and Photoluminescence Spectroscopy of Single-Walled Carbon-13 Isotope Nanotubes

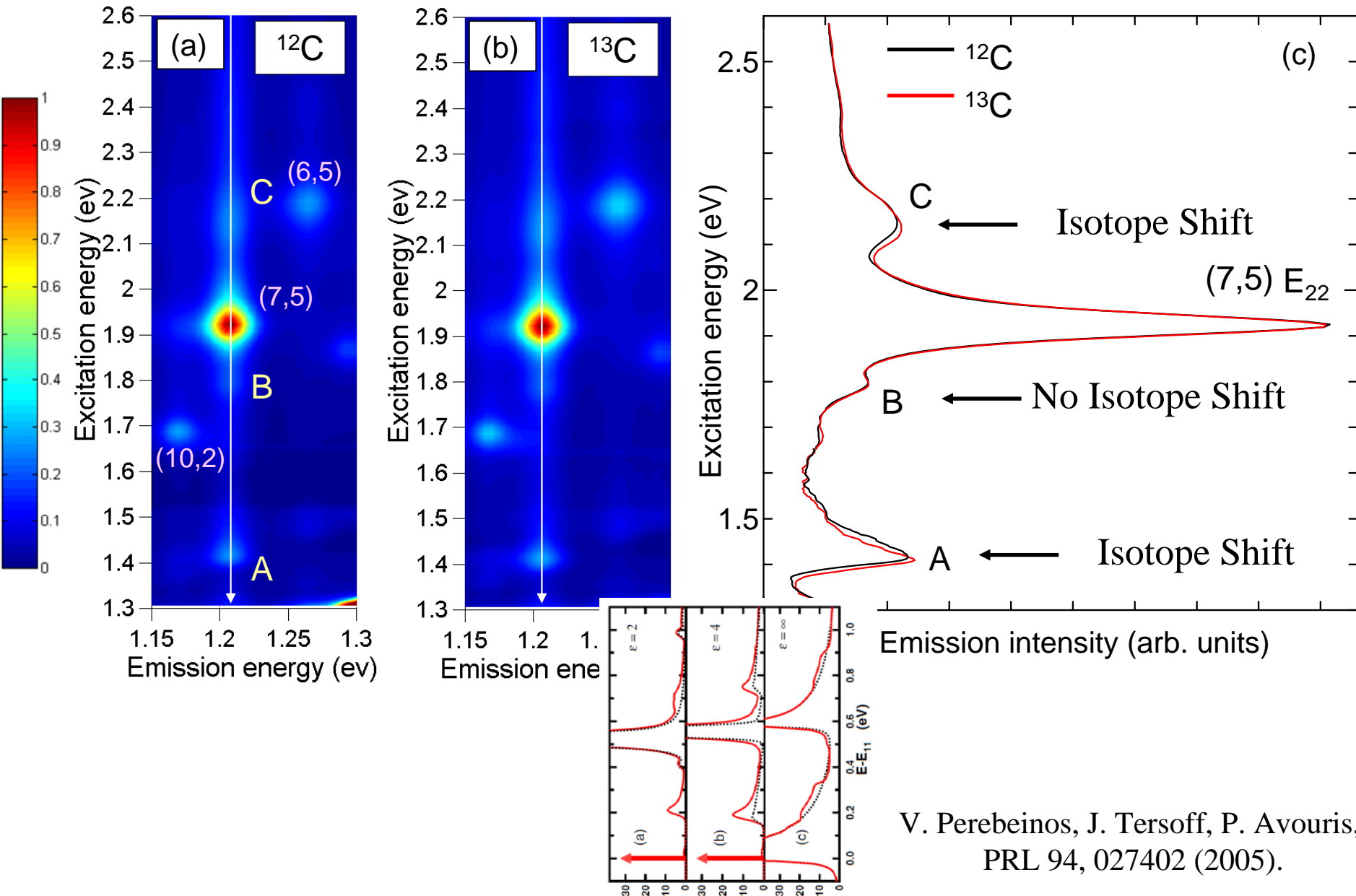
I.69

Shigeo Maruyama and Yuhei Miyauchi

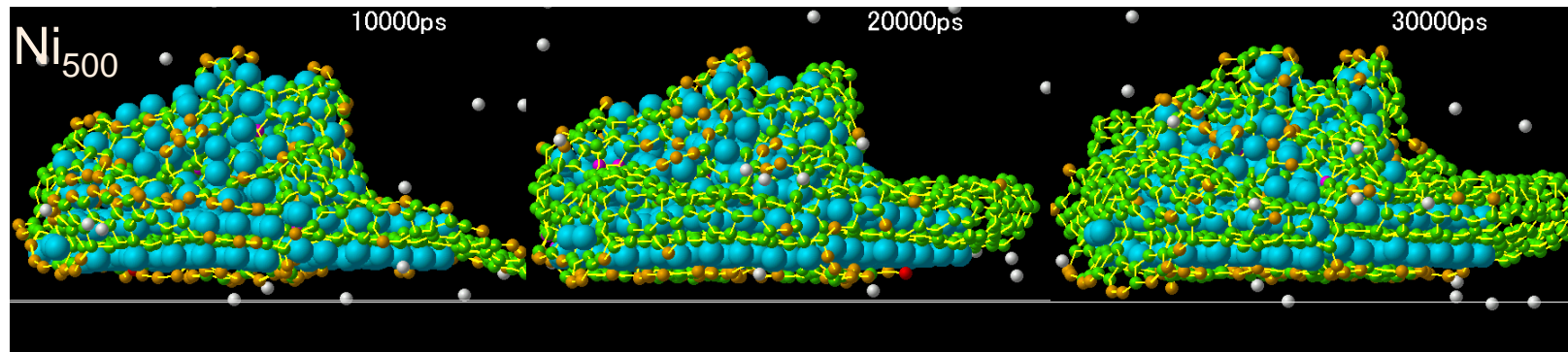
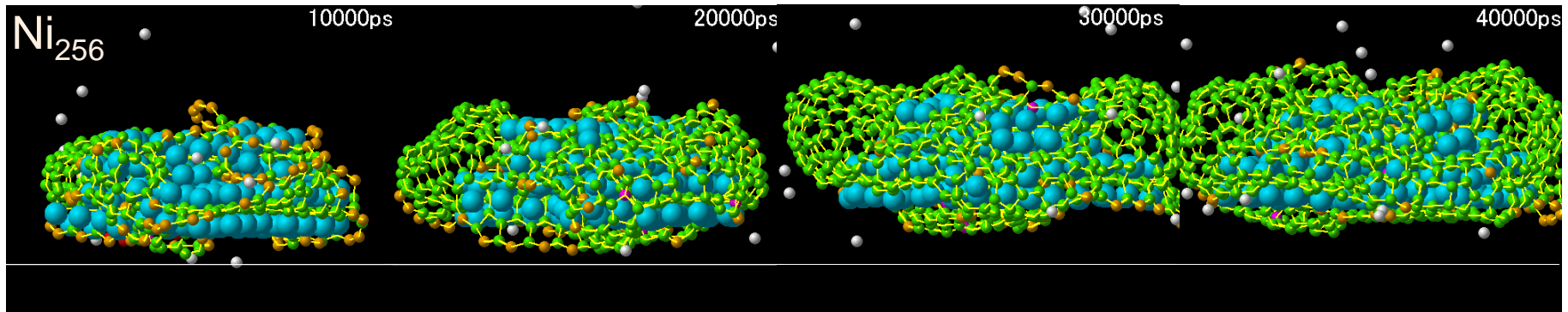
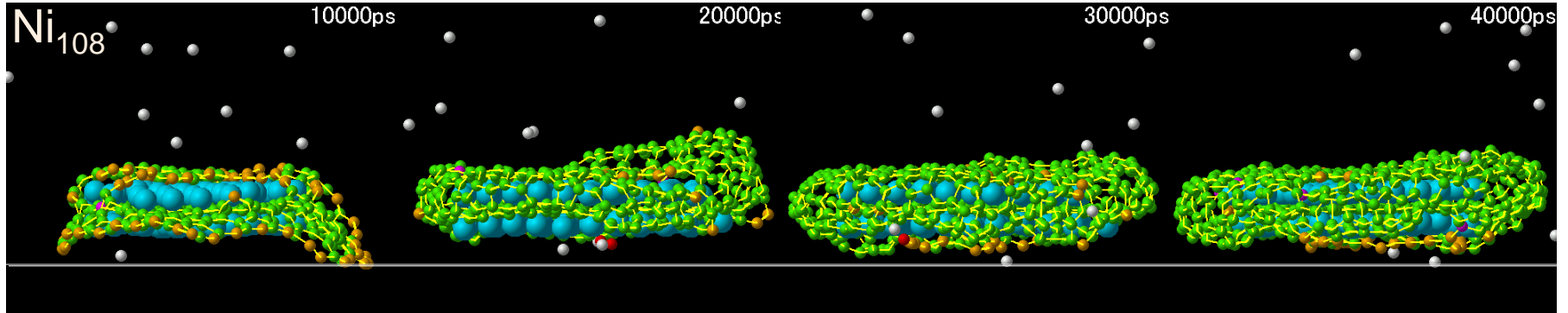
Dept. of Mech. Eng., The University of Tokyo



# PLE Spectra of SW<sup>13</sup>CNTs

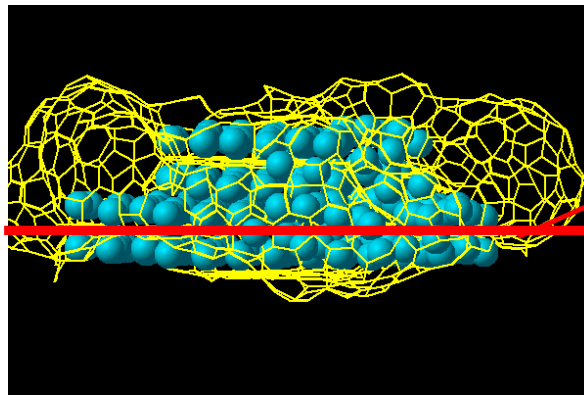


## MD of Nucleation of SWNTs from a Cluster on a Substrate

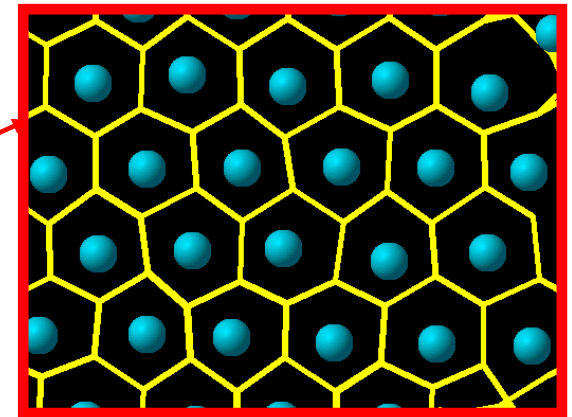


## Cross Sectional View of the Metal Cluster

$\text{Ni}_{256}$ ,  $D_e = 0.98\text{eV}$   
40 ns, 2500K

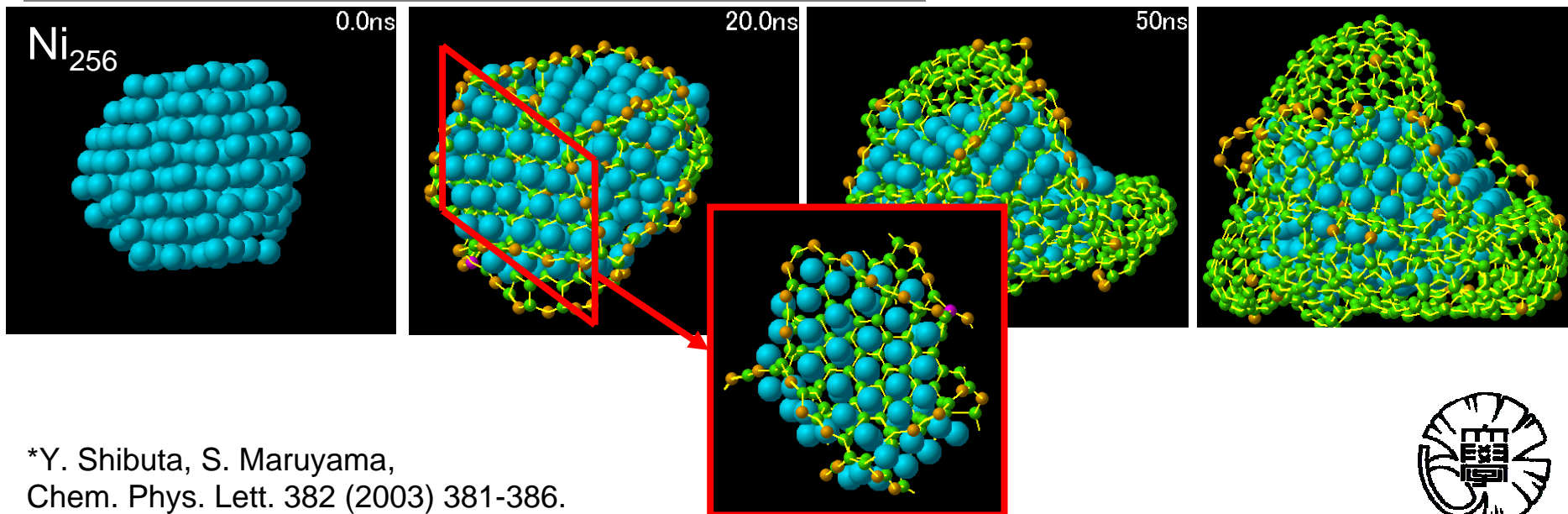


Carbon atoms are not shown for clarity.



Ni(111) structure

Comparison with the **non-supported** cluster\*



\*Y. Shibuta, S. Maruyama,  
Chem. Phys. Lett. 382 (2003) 381-386.



## Yet Open Issues

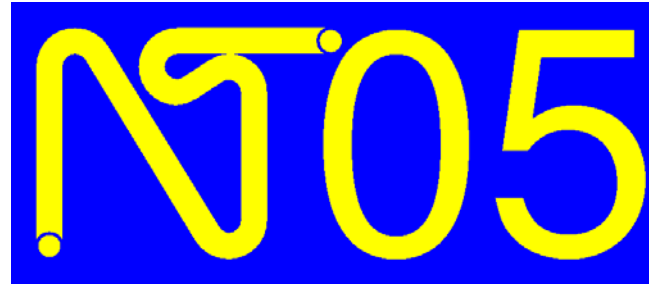
- \* **Synthesis of (n,m) controlled SWCNT's**
- \* **Nucleation and growth mechanisms of SWCNT with given (n,m)**

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**A.3 Marcos Pimenta**

**Tuesday, June 28**

## **Section II - Non-CVD nanotube synthesis**

II-1 to II-8 downstairs, II-9 to II-20 in this level

## **Section III – Formation and characterization of unusual nanostructures**

all posters in this level

## **Section IV – Raman characterization of nanotubes** all all posters in this level

**Marcos A. Pimenta**

**Departamento de Física, UFMG**

**Belo Horizonte, Brasil**



## Section II - Non-CVD nanotube synthesis (16 posters)

- Chirality control – CNT chirality determined by the atomic structure of the SiC substrate (II-15)
- Isolated nanotubes made by arc-discharge (II-2)

### Influence of catalyst, promoter and electrodes

- Ni and Y carbonates and oxides (II-6)
- Different transition and rare earth metals (II-16)
- Influence of sulfur promoter (II-14)
- Influence of graphite electrodes (II-8)
- Pre-formed catalyst: NT diameter determined by catalyst size (II-4)
- Real-time study: diameter does not depend on particle size (II-17)

## New Methods

- Wet chemical synthesis: cyclacene (II-10)
- Spray pyrolysis of natural precursors (II-7)
- Radio frequency magnetron sputtering (C and BN) (II-5)

## Formation Mechanisms

- Fluorescence experiments (laser vaporization method) (II-11)
  - Arc discharge (II-9)
  - BN bamboo-like nanostructures (II-20)
- 
- Large scale production: DWNTs (II-12), MWNTs (II-18)  
carbon cones and carbon disks (II-18)
  - Long amorphous carbon nanotube ropes (21 cm) (II-1)

## **Section III – Formation and characterization of unusual nanostructures (14 posters)**

- Controlled assembling nanotubes on surfaces with atomic steps (III-12)

### **Things @ Nanotubes**

- Fluid Ice (Neutron scattering) (III-3)
- Ice nanotube (X-ray diffraction) (III-14)
- Magnetic nanoparticles (III-11)

### **Nanohorns, Nanocapsules, Nanofibers, Nanoribbons**

- Desorption of organic materials on nanohorns (III-7)
- Metal-encapsulated nanohorns and nanocapsules (III-5, III-8)
- Growth and characterization of nanofibers (III-4, III-10)
- Conversion of nanotubes into nanoribbons (III-9)
- Simulation of carbon deposit in zeolyte nanopores (III-2)

# Section IV – Raman characterization of nanotubes (11 posters)

SWNTs (7), DWNTs (2), MWNTs (1)

## SWNTs

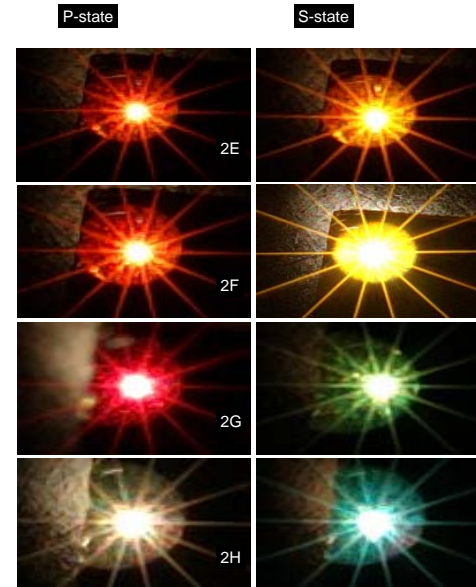
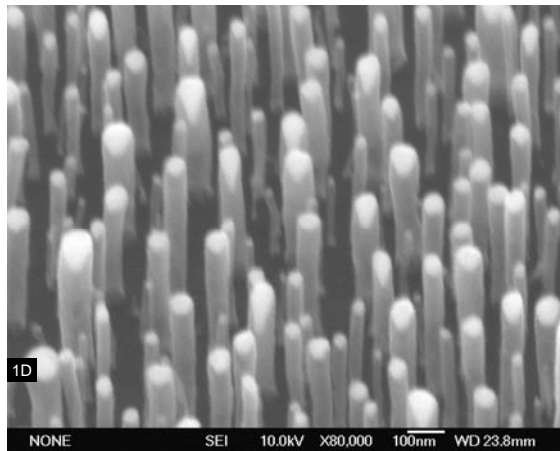
- Correlation between Raman and transport measurements (IV-3)
- UV Raman in SWNTs @ zeolites ( $d_T = 0.3$  nm) (IV-10)
- Comparison of NTs on Si/SiO<sub>2</sub> surfaces and in aqueous solution (IV-2)
- Raman and electrochemical doping (IV-8)
- Temperature dependence (4-1000K) of the Raman spectra (IV-12)
- Calculation of the RBM resonant profile for 300 SWNTs (IV-1)
- Infrared modes (purification and annealing of the sample) (IV-7)

# DWNTs

- Fine structure of RBM – inner tube inside different outer tubes (IV-5)
- Raman under pressure – inner tubes protected by outer tubes (IV-9)

# MWNTs

- Vertically aligned – Ag coated for SERS (IV-6)

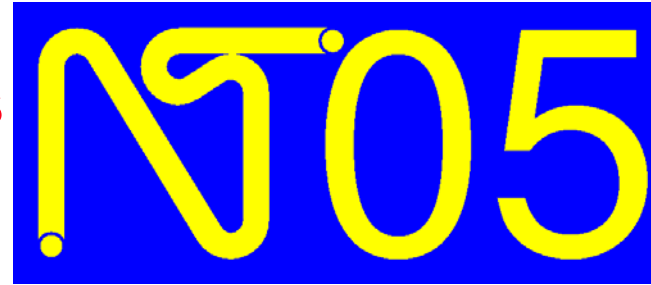


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**A.4 Jack Fischer**

**Tuesday, June 28**

# Sixth International Conference on the Science and Application of Nanotubes

Göteborg University, Chalmers University  
of Technology and University College of Borås  
June 26-July 1, 2005 (Gothenburg, Sweden)

## ***“CHEMICAL” POSTERS***

- **V . Characterization of Nanotubes (18)**
- **VI. Nanotube Dispersion and Purification (9)**
- **VII. Chemical Modification of Nanotubes (29!)**
- **VIII. Non-Carbon Nanotubes (12)**

# V. Characterization of Nanotubes

- **Individuals**, ropes & bundles, **fibers, films**, suspensions/dispersions, composites
- **(n,m) determination and synthetic control**
- **density, porosity, preferred orientation**
- **Atomic-scale defects – more emphasis and new techniques needed!**

Technique mentioned most often: HRTEM, followed closely

by optical probes (absorption, PL)

“New” techniques: NEXAFS - chemically-specific orientation information

SAXS – structure of large aggregates

Popular “problems” in characterization:

purity determination/quantification

tuning and measuring chirality

nitrogen (sidewall) doping

gas sorption

New issues in characterization:

radiation effects on tubeFET behavior,

high pressure phenomena



# VI. Nanotube Dispersion and Purification

- How pure is pure enough? Depends on application.
- Would it be easier/better to grow them pure in the first place? How? Catalyst tricks? MWNT easier to grow relatively pure.
- Dispersion: precursor to **i) rational or self-assembly into higher-order structures, e.g. fiber spinning, thin film deposition; ii) sorting by (n,m) and nanodevice engineering; iii) composite processing; .....**
- Can it all be done without damaging tubes (sonication, sidewall adducts..) ?

## 9 ABSTRACTS

- Reference standards for “pure” SWNT.
- Drift of SWNT in DC electric field during growth – diagnostic of CVD yield
- Novel SWNT dispersants based on saccharide chemistry.
- Heat treatment and opening ends to facilitate peapod formation.
- Dispersing LONNNNNNNNNNNNG MWNTs and composite synthesis.
- Bundle/rope dissociation by amides: “SWNT causes rearrangement of solvent” (theory and expt.). See also P23 (X.1) “partly ordered solvent around acid-swollen SWNT fibers” (WZ and JEF).
- Diameter-selective oxidation by hydrogen peroxide.
- Patterned SWNT deposits on the anode in DC electrophoresis using aqueous electrolyte.

# VII. Chemical Modification of Nanotubes

- Functionalization: solubility, separation, tube-matrix adhesion ( 8)
- Doping/intercalation/filling (5)
- Control surface chemistry; curvature; adsorption sites (4)
- DNA hybrids (3)
- Fluorination (3)
- Sensor applications (2)
- Nitrogen doping (2)
- Purification, esp. removal of amorphous carbon (1)
- Cutting and sorting by length (1)
- Sidewall defects: measure and chemically modify (1)
- Nanotube/nanoparticle hybrids (1) (see also I.46)

$\Sigma(n) > \#$  posters  
Theory and experiment  
Overlap with posters VI.

## VIII. Non-Carbon Nanotubes

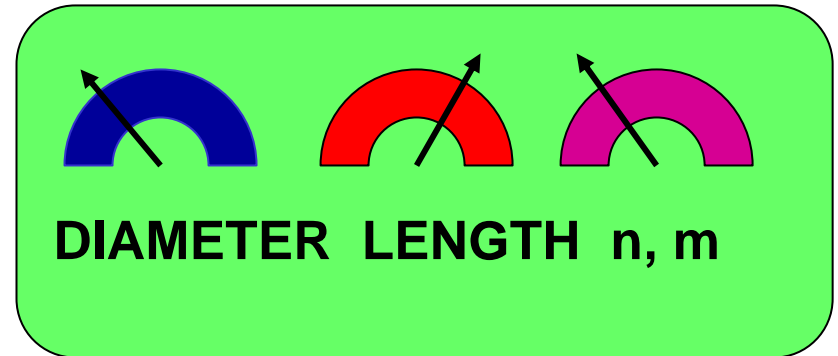
- Point and line defects in BN nanotubes (theory)
- Synthesis of BN nanotubes by *in-situ* nitriding
- BN SWNT synthesis & mechanism: EELS, optical properties
- Vertically-aligned BN tubes by PE-PLV @ 600C
- Boron sheets and tubes: structure, el.props., H<sub>2</sub> sorption (thy)
- Si nanoparticles and nanowires: synthesis, low T transport
- TiO<sub>2</sub> nanotubes -> nanoparticles; chimie douce
- Bismuth sulfide nanotubes @ 350C
- Mo<sub>6</sub>S<sub>4.5</sub>I<sub>4.5</sub> NW bundles: solubility, structure & mech.props.
- Aligned ZnO NW on patterned substrates; PL spectra

# What's missing? What's next?

- V. Characterization of Nanotubes (18)
- ~~VI. Nanotube Dispersion and Purification (9)~~
- VII. Chemical Modification of Nanotubes (29!)
- VIII. Non-Carbon Nanotubes (12)

Continuous large-scale growth of isolated, perfect CNT's

“Designer” CNT synthesis



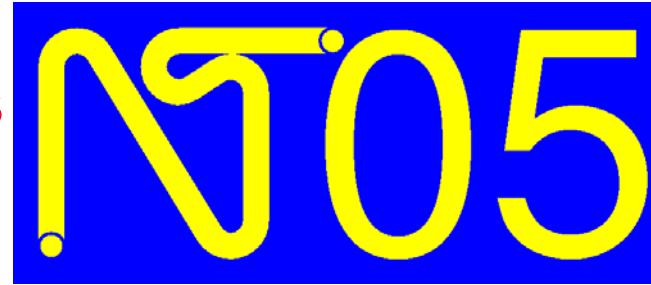
Single-tube *in situ* physical property measurements ( $\rho, \kappa, \epsilon, \alpha, \dots$ ) concurrent with atomic-scale structural and defect diagnostics – HRTEM appears to be the only option. (limitations of Raman, scanned probe, .....

**NT05: Sixth International Conference on the  
Science and Application of Nanotubes**

***Göteborg, Sweden***

***June 26 - July 1, 2005***

**<http://nanotube.msu.edu/nt05/>**



**B.1 Pavel Nikolaev**

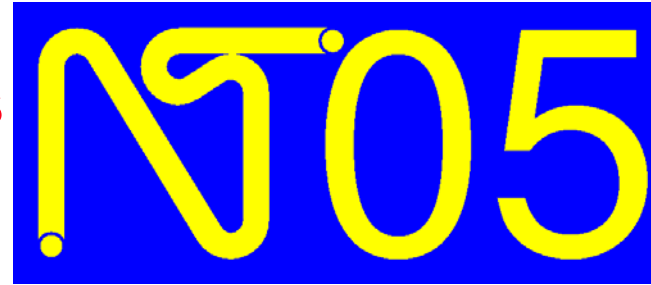
**Thursday, June 30**

**NT05: Sixth International Conference on the  
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**B.1 Pavel Nikolaev**

**Thursday, June 30**

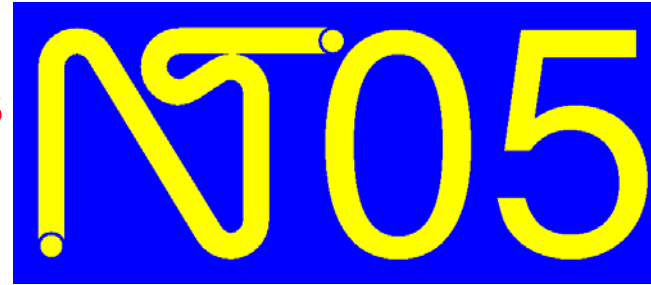
**Slides not yet received**

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**<http://nanotube.msu.edu/nt05/>**



**B.2 Apparao Rao**

**Thursday, June 30**

Poster Session XI

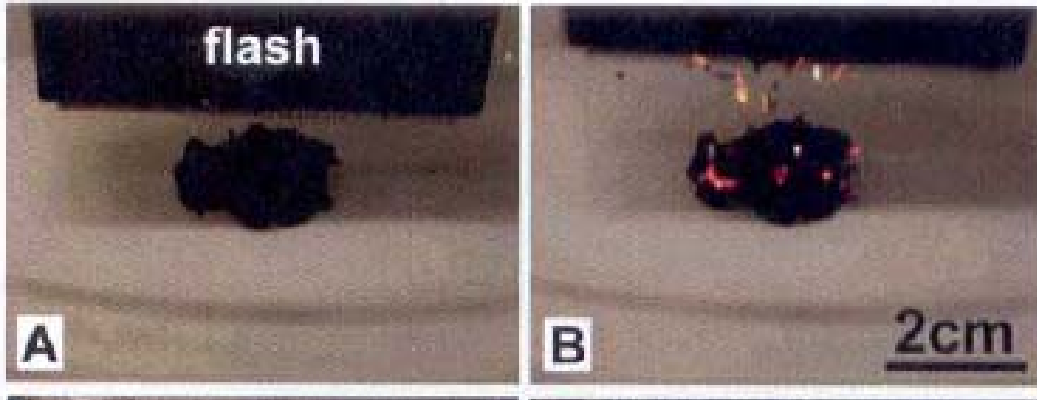
Poster Session XII

Poster Session XIII



# Poster Session XI

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Optical Ignition of CNT-doped Energetic Materials

-SWNTs when exposed to conventional photographic flash spontaneously ignite

Important practical benefits: **(XI. 1)**

(1) the optical signal is immune to electromagnetic interference, ambient conditions of pressure and temperature,

(2) pulse-delivery is not dependent on materials that might degrade over time.

# Poster Session XII

---

(5 Computational, 12 Experimental)

Elastic properties of CNTs as a function of:

- length, outer / inner tube diameter (1), chirality (11), interaction with substrate (13)
- coiled NTs (14, 16)
- precursors used in the synthesis (4, 16)
- MoS<sub>2</sub> NTs (3), BN nanowires (10), polypyrrole NTs (12)

# Poster Session XII

---

How mechanical properties influence electronic properties? (2)

Current induced bends, repairing structural defects (5,6)

Selective removal of individual CNTs from a high density CNT network (7)

Cantilevers – zeptogram (8), attogram (14) mass detection

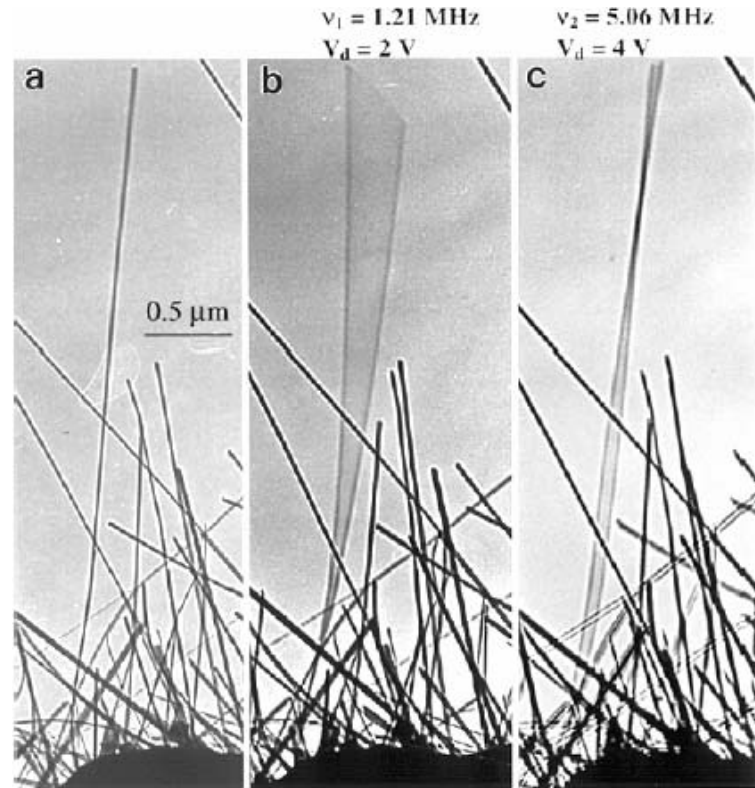
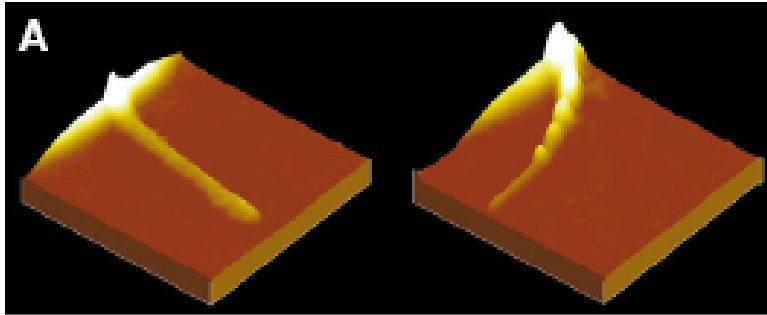
Suspended tubes

- evidence for phonon-assisted tunneling (15)
- thermal effects on optical transition energies  $E_{22}$  (17)

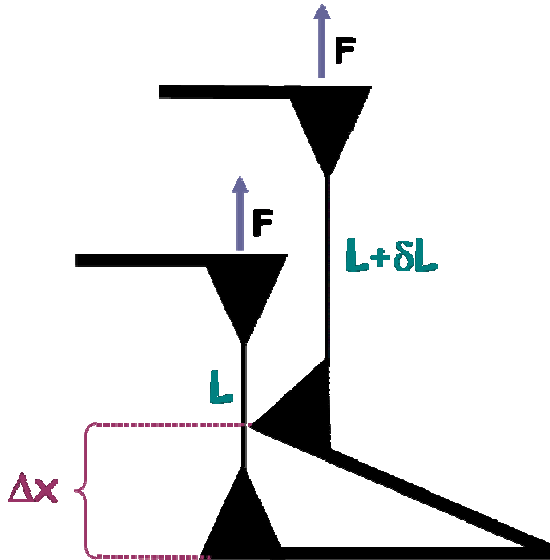
Anisotropic heat transfer by CNTs (9)

# Methods for Measuring Bending Modulus

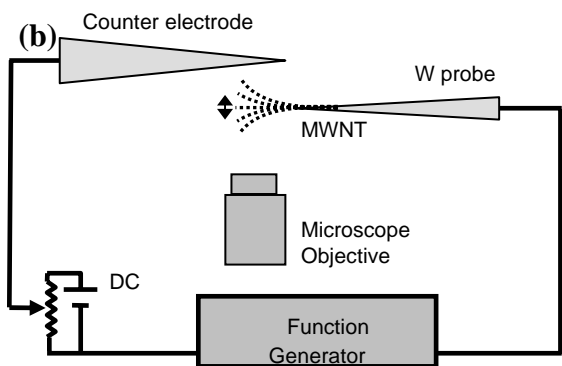
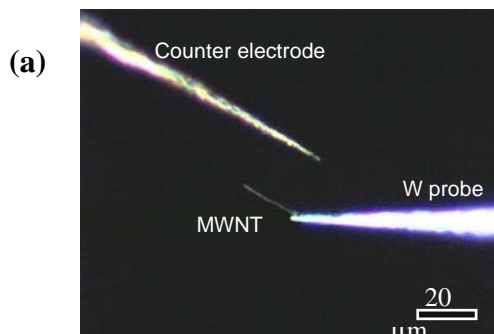
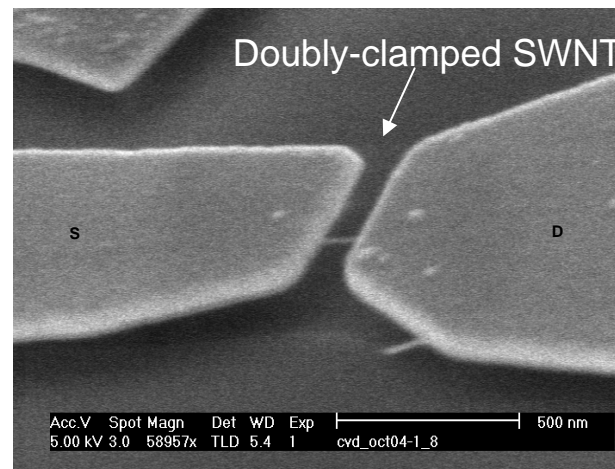
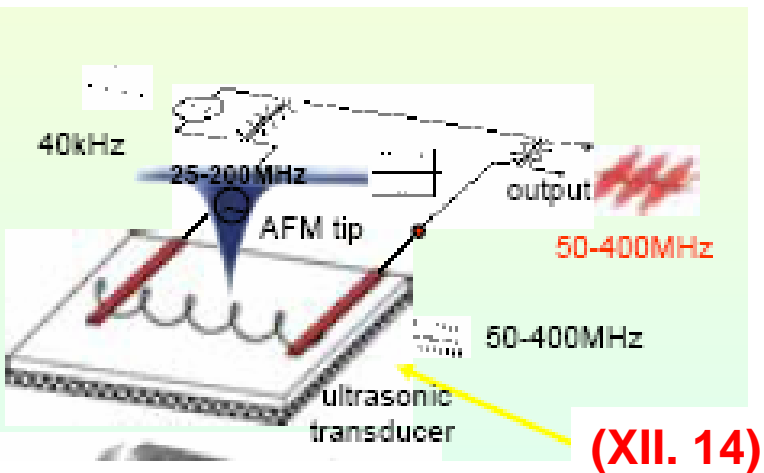
Wong et al. *Science* **277**, 1971 (1997).



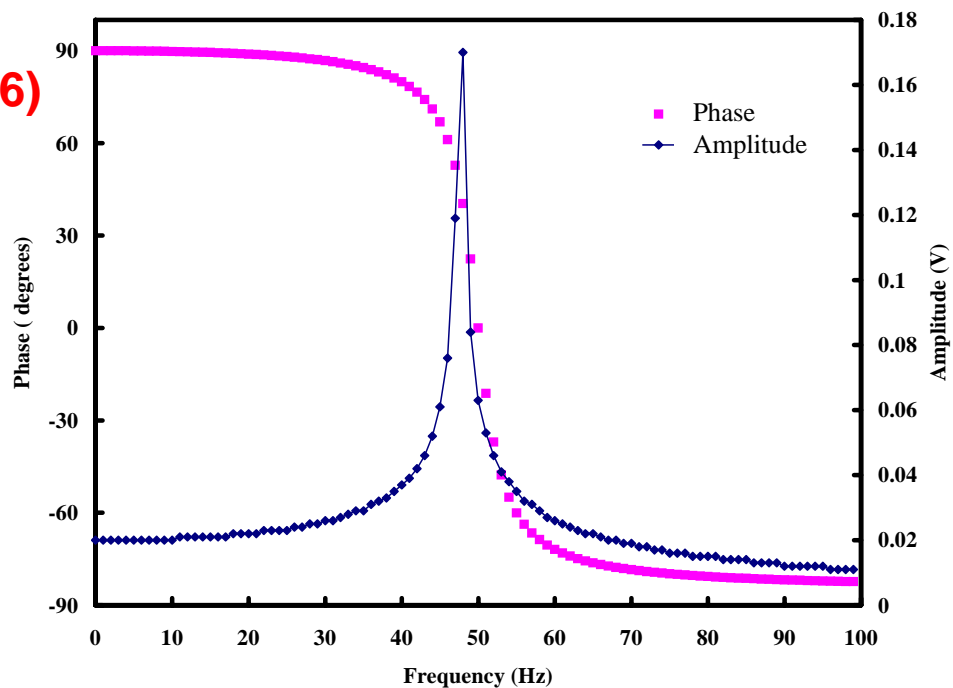
Wang et al. *Pure Appl. Chem.*, Vol. 72, Nos. 1–2, pp. 209–219, 2000.



# NEMS



**(XII. 16)**

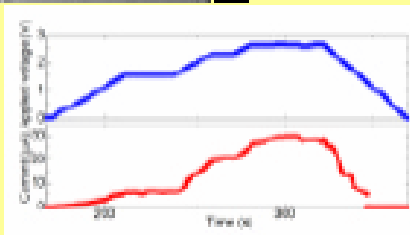
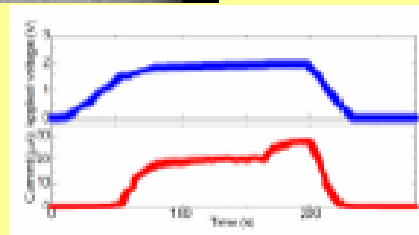
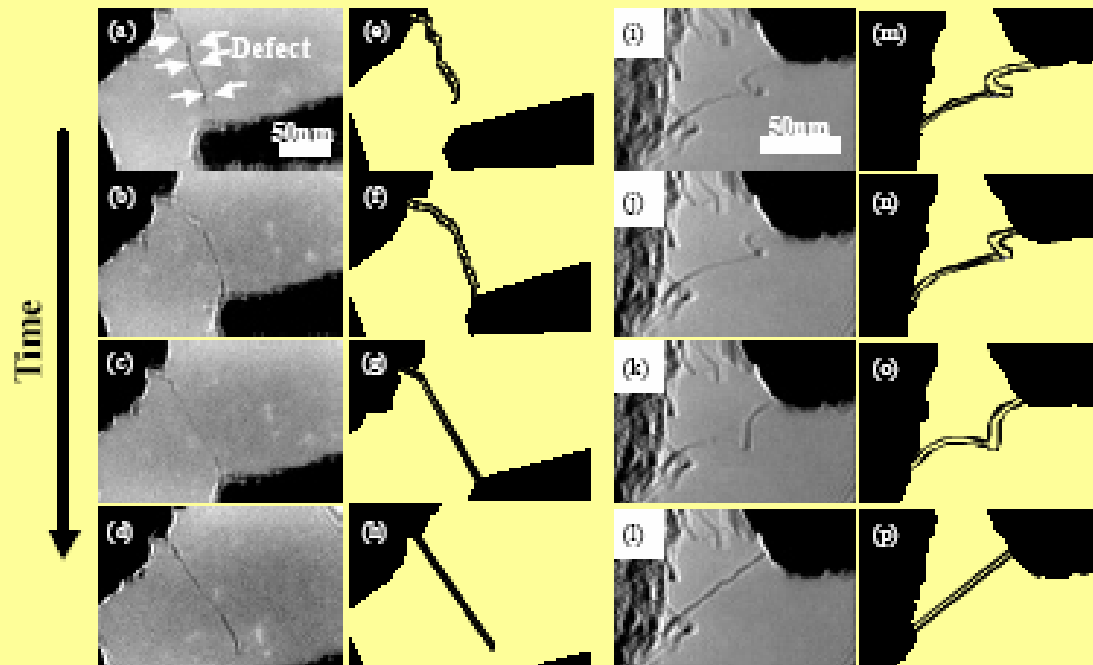


## XII. 5

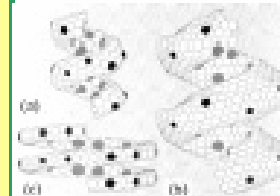
### The generation and disappearance of the SW defects

#### A waved DWCNT

#### A coiled DWCNT



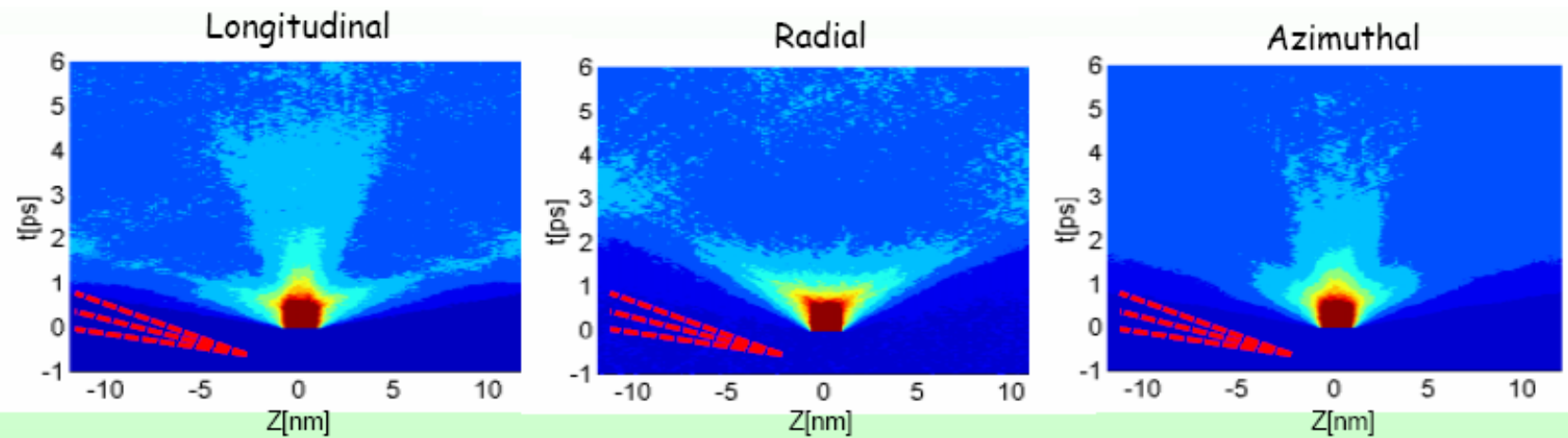
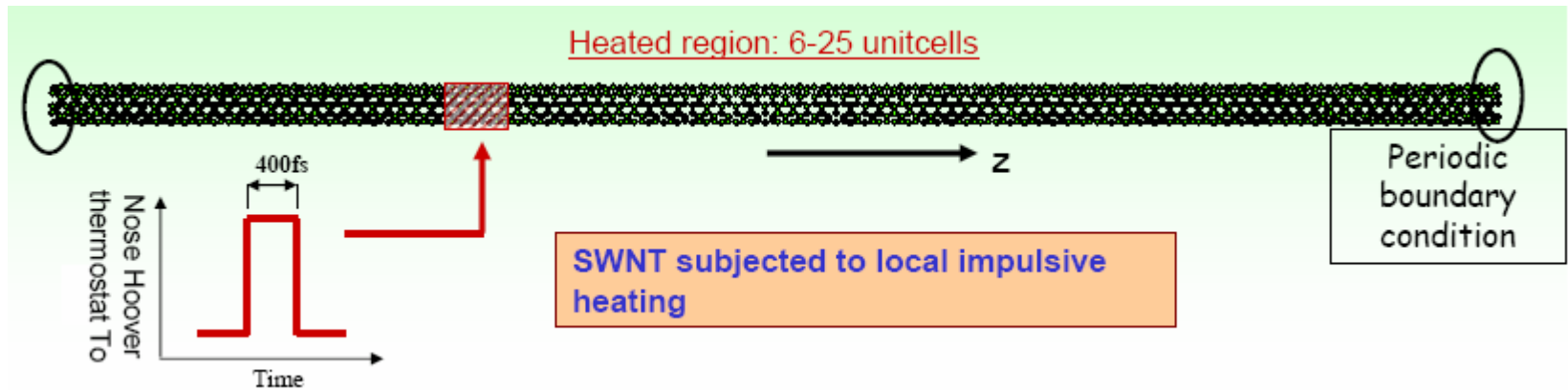
**These results are proof for the restoration of defects on CNTs by heating due to flowing current.**



The coiled carbon nanotube has the pentagons and heptagons for the outer and inner ridge lines of a coil, respectively.

S. Iijima, S. Iijima and J. Shimokawa, Phys. Rev. B 48, 5643 (1993).

# XII.9



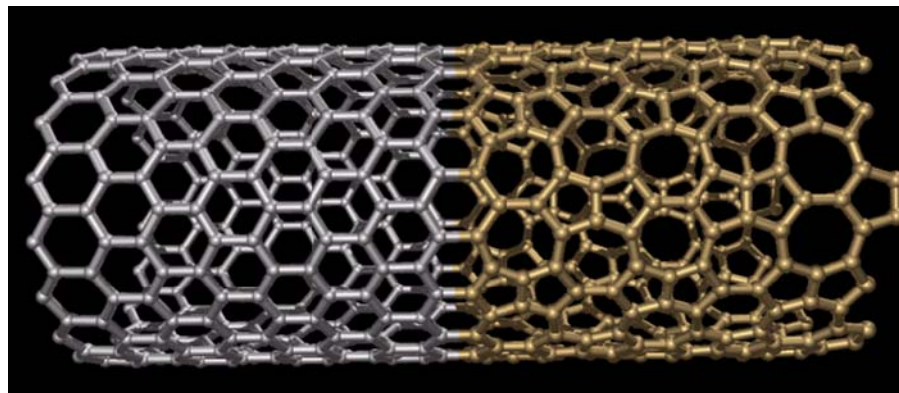
# Poster Session XIII

---

(6 Computational, 4 Experimental)

## Atomic Structure of NTs

- Identical chiralities in a single DWNT inside a DWNT bundle (1)
- Effect of HTT on the interlayer spacing between adjacent graphene layers inside a MWNT (3)
- Computed powder diffraction pattern for Haekelelite CNTs (4,5)





# Poster Session XIII

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(6 Computational, 4 Experimental)

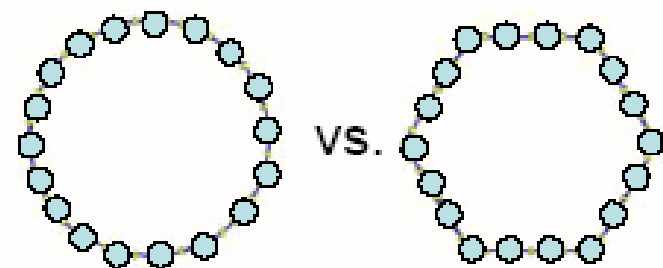
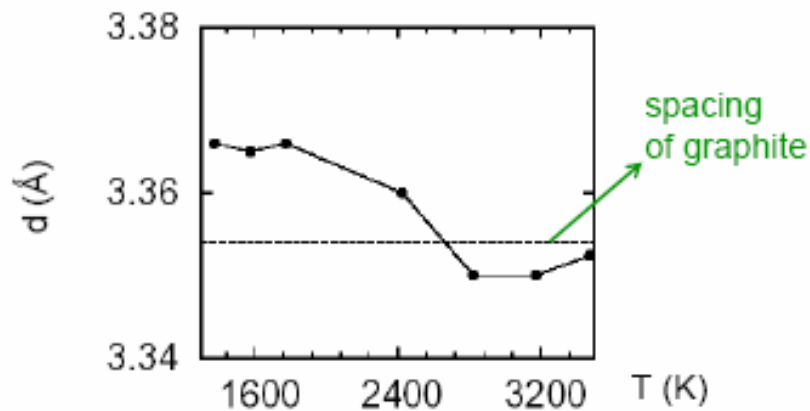
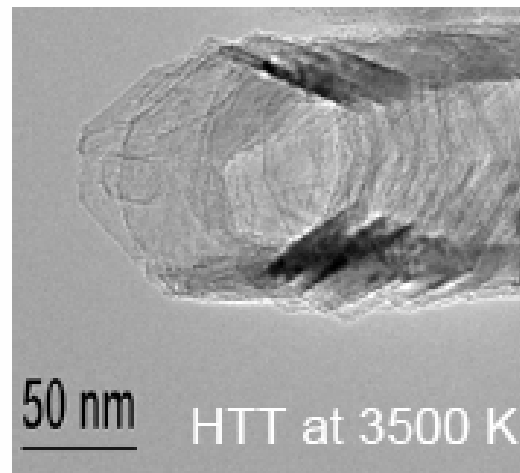
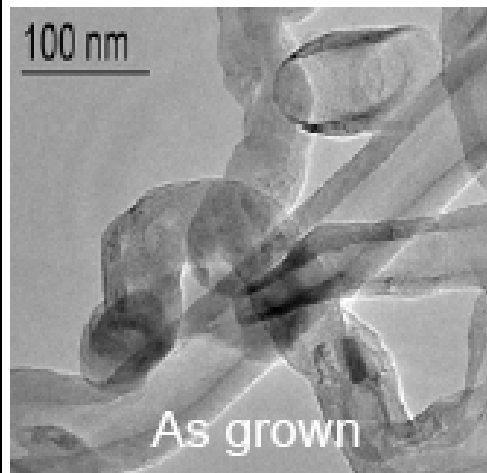
## Atomic Structure of NTs

- Controlled point defects and its mobility (6)
- Correct description of molecular interactions in peapods (7)
- Near Edge X-ray Absorption Fine Structure (NEXAFS) for determining the dopant concentration (9)
- Peierls distortion in small diameter tubes (2, 8, 10)

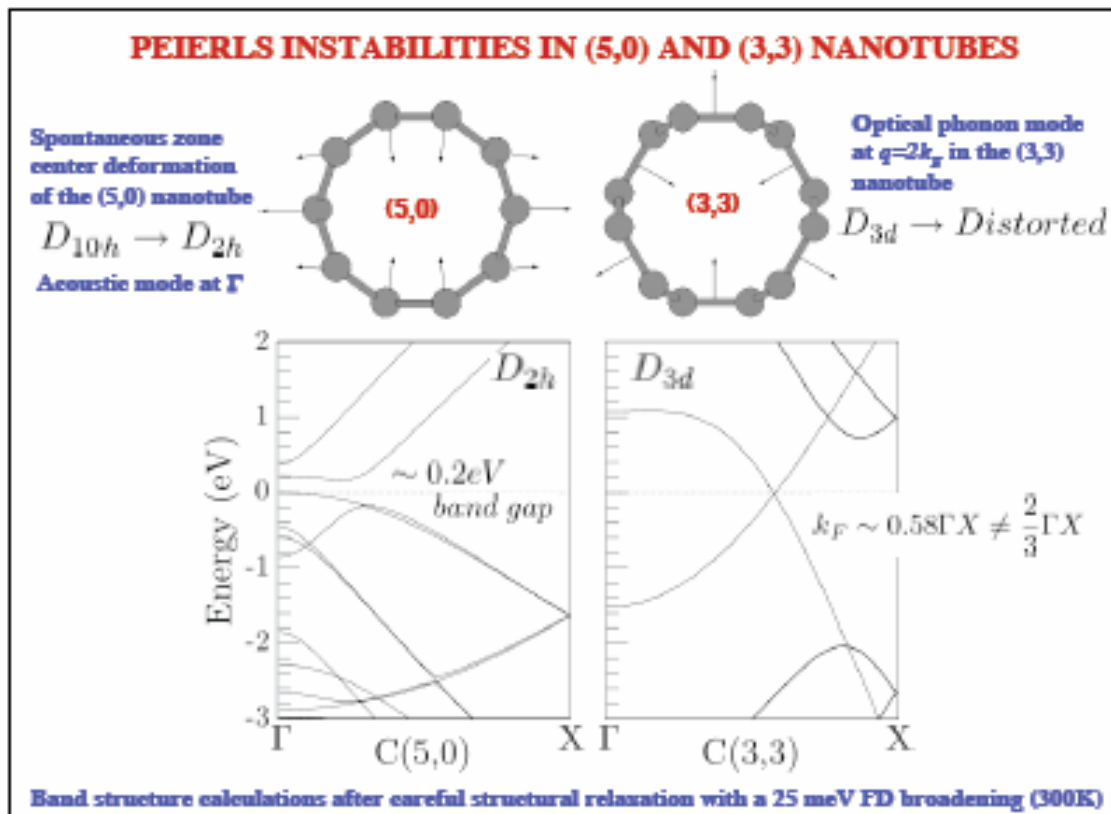
# XIII.3

## Experimental Confirmation

### Transmission Electron Microscopy



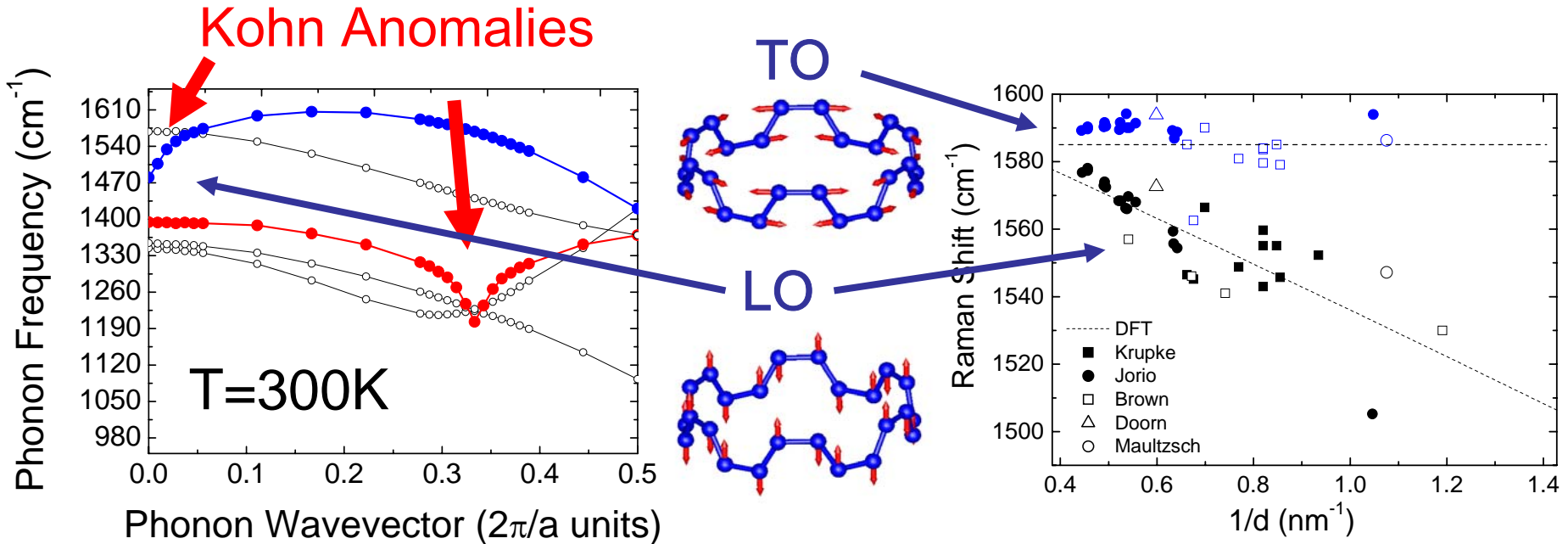
## XIII. 2





# XIII.10: Kohn Anomalies and Temperature Dependent Peierls Distortions in Nanotubes

S. Piscanec, M. Lazzeri, F. Mauri, A. C. Ferrari, J. Robertson



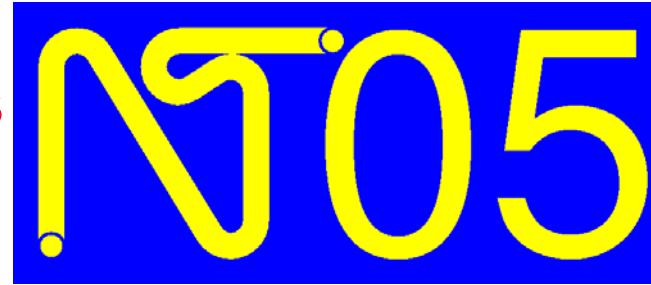
- Efficient DFT calculation of phonon dispersion of large diameter nanotubes
- Study of Kohn anomalies, Peierls distortion and LO-TO splitting in metallic tubes
- Peierls Distortion temperature exponentially depends on diameter, and is negligible for tubes normally used in experiments ( $\ll 1\text{K}$ )

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**B.3 Tony Heinz**

**Thursday, June 30**

# Overview of Poster Session XIV

## Transport in Nanotubes

Tony Heinz

Columbia University

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# Desired Presentation







# Realistic Presentation



Horse Guards Parade

Buckingham Palace

Playground

Lavatories



Guards Museum

# Actual Presenter



# Transport in Nanotubes: Session B3 / Poster in group XIV

- Electrical Transport: 28
- Mechanical and electro-mechanical: 5
- Thermal and thermoelectric: 2
- Material (atom transport): 1

# Electrical Transport

- Ideal structures: Mechanisms, noise, as quantum dots
- Exotic regimes: Tomonaga-Luttinger liquids (TLL), superconductivity
- Perturbations: Defects, adsorbates, etc.
- Behavior of contacts
- New structures and materials

# Electrical Transport: Ideal Structures

- XIV36E Transport in long suspended nanotubes; Influence of strain (straight/bent)
- XIV28T Role of hot phonons for transport in SWNTs
- XIV10E Shot noise in SW/MWNTs and spectral characteristics
- XIV18E Noise in SWNTs as random telegraph process
- XIV27T Quantum Dots of SWs under magnetic field
- XIV29E Photon assisted tunneling in SWNT QD
- XIV38T Two coupled QD defined by gates on SW

## Poster XIV.28

### **Electron Transport and Hot Phonons in SWCNTs**

**M.Lazzeri, S.Piscanec, F.Mauri, A.C.Ferari, J.Robertson**

Several transport measurements in metallic SWCNTs report a scattering length of  $l_{\text{scatt}} \sim 15\text{nm}$  (at high bias).

We show that this length might be in contrast with other electron-phonon coupling measurements (IXS-phonon dispersion, phonon line-width, ...)

#### **Proposed Explanation:**

**During electron transport, phonons are very hot !**

**( $T_{\text{eff}} \sim 6000\text{ K}$ )**

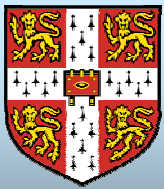
# Electrical Transport: Exotic Regimes

- XIV5E Superconductivity end-bonded MWNTs at 12K
- XIV25E SWNT contacted to superconductors (SMS)
- XIV6E Tomonaga-Luttinger liquid behavior in peapod (with  $C_{60}$ ) SWNT
- XIV12E Photoemission of peapod SWNTs (with K and  $C_{60}$ ) to study TLL behavior
- XIV13T TLL behavior, diamagnetism in SWNTs
- XIV16T Conductivity in SWNT networks
- XIV30T SWNT conductivity for high B field, theory

# Electrical Transport: Role of Perturbations from Defects and Adsorbates

- XIV1E      Effect of annealing on MWNT transport
- XIV34E     Influence of doping of metallic SWNTs
- XIV31T     Conductance in zigzag/chiral metallic SWNTs with defects
  
- XIV21T     SWNTs w/ many defects: Anderson localiz.
- XI26E      Tunneling spectrosc. on disordered MWNTs
  
- XIV2T     |      Influence of adsorbates on electronic structure
- XIV17T    |      and charge transport characteristics





# Breakdown of ballistic transport in zigzag and chiral metallic nanotubes



S. Povia<sup>1</sup>, S. Reich<sup>1</sup>, P. Ordejón<sup>2</sup>, A. C. Ferrari<sup>1</sup> and J. Robertson<sup>1</sup>

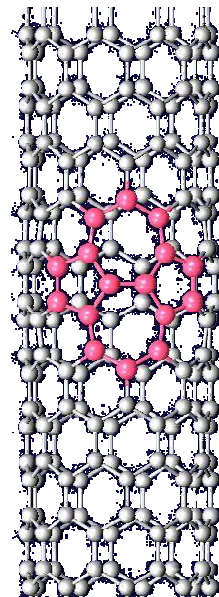
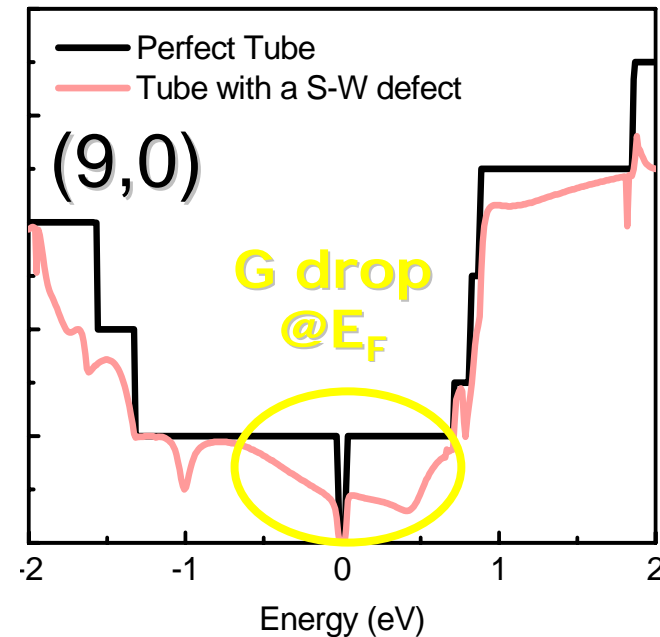
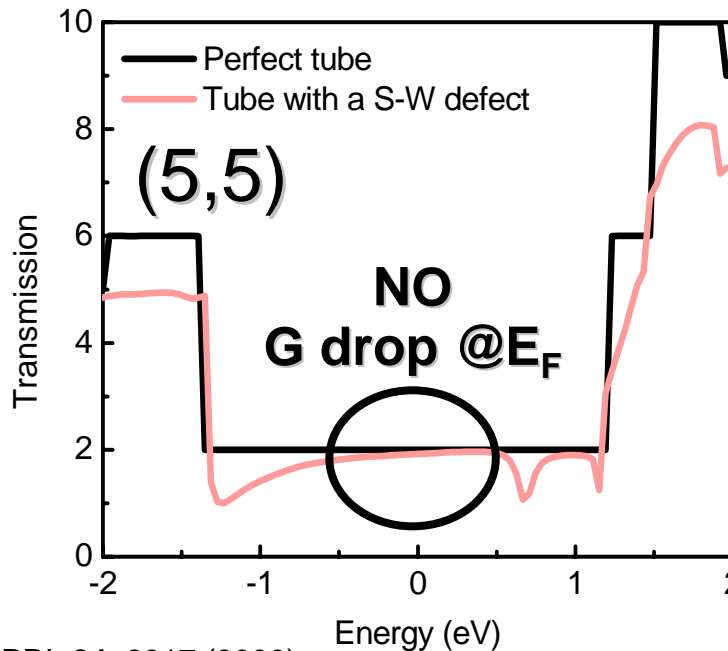
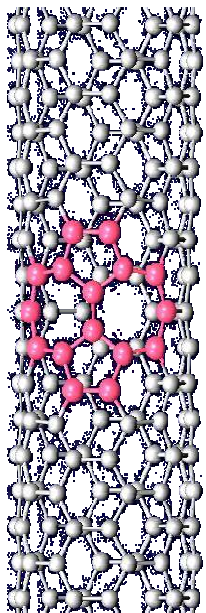
<sup>1</sup> University of Cambridge, UK <sup>2</sup> Institut de Ciència de Materials de Barcelona, Spain

## Poster XIV.31

### Insertion of a Stone-Wales defect: **conductance @ $E_F$ ? IV?**

So far: armchair

This work:  
**zigzag and chiral** conductance @ 0eV  
+ **calculated IV**



# Electrical Transport: Contacts

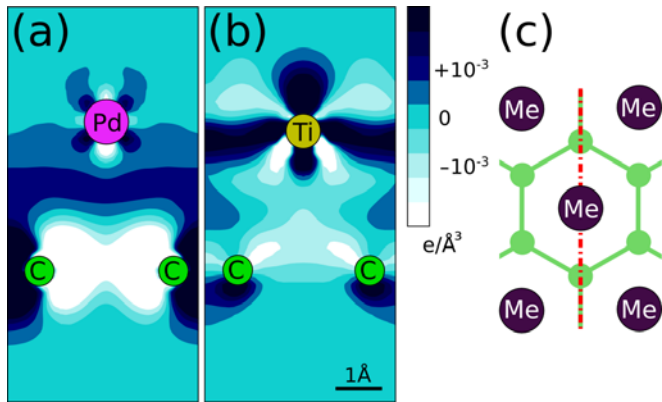
- XIV4E     Contacts SWNTs by AC properties
- XIV35E     Schottky barriers for high freq.;  
also high current field emission
- XIV15E     SWNT length dependence; deduce  
contact resistance
- XIV39T     Theory of metallic contacts

# Contact dependence of carrier injection in carbon nanotubes: an *ab initio* study

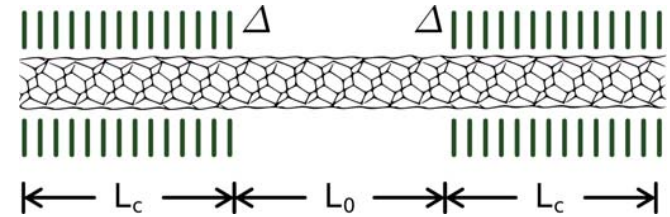
XIV.38

Norbert Nemeč, David Tománek and Gianaurelio Cuniberti

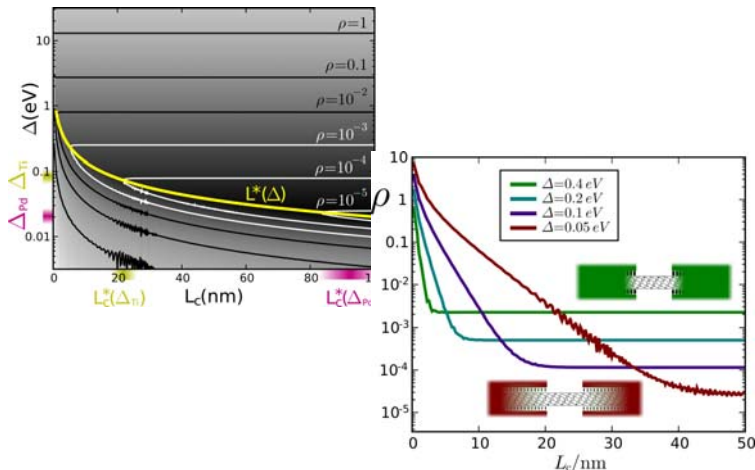
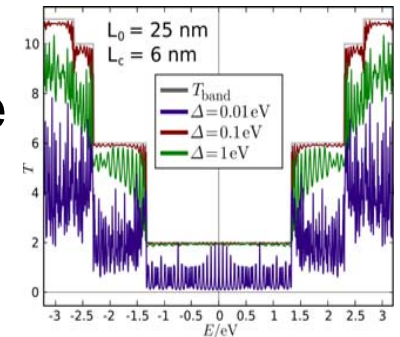
## Microscopic *ab initio* study



+



Large-scale model calculation



strong coupling = bad contact  
weak coupling = transparent contact

# Electrical Transport: New Structures and Materials

- XIV9T Transport properties of 3-terminal SWNT junctions (substitute for original poster)
- XIV19E Loop SWNT structures: charging behavior
- XIV32E Transverse electrical conductivity on MWNT
- XIV20E GaAs / CNT hybrids by MBE fabrication
- XIV14T Gold nanotubes formed from gold nanobridges: theory of structure, transport

# Mechanical and Electromechanical Properties (Also many in other sessions)

- XIV7T Electromechanical instability of suspended SWNTs
- XIV17E Three terminal nanotube relay with MWNTs
- XIV24T/E Electrostatic deflection of MWNT
- XIV35E Mechanical switches with SWNTs
- XIV36T Stepper motor simulation using torroidal CNTs

# Thermal and Thermoelectric Properties

- XIV3E Thermal transport in individual MWNTs/ bundles; correlation with electrical
- V19E Bolometers and electron cooling in S-I-Nanotube junctions

# Mass Transport

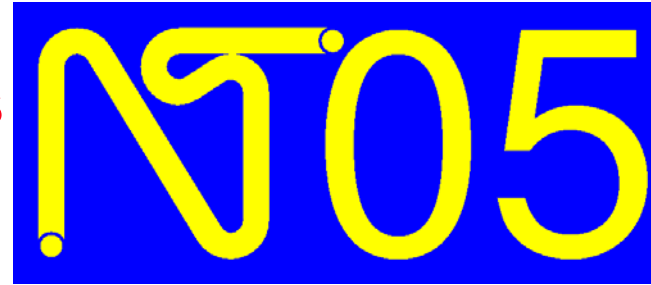
- XIV33E      Nanopipettes in MWNT:  
Electromigration in tubes filled with iron atoms

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**B.4 Gianaurelio Cuniberti Friday, July 1**



# Overview on NT05 poster session B3 (categories: XV, XVI, XVII, XVIII)

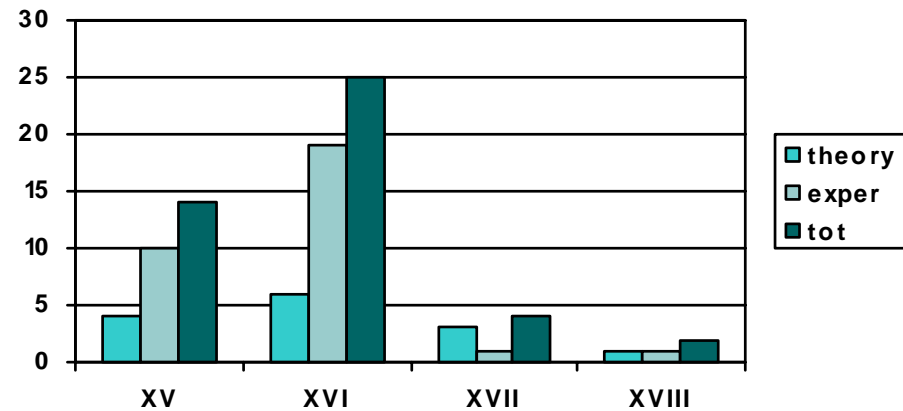
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G. Cuniberti  
University of Regensburg (DE)





# Categories



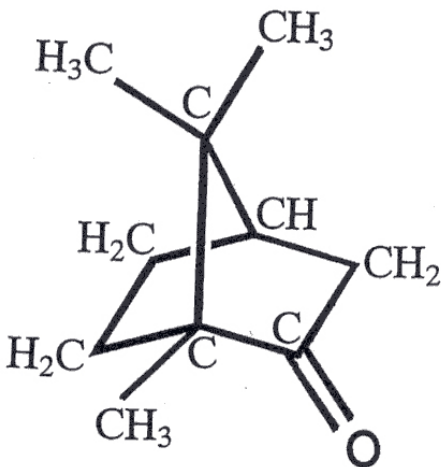
- XV. Field Electron Emission (**14**)
- XVI. Optical Properties and Optoelectronics (**24+1**)
- XVII. Transport in Complex Nanostructures (**4**)
- XVIII. Electron-Phonon Coupling in Complex Nanostructures (**2**)

## XV. Field Electron Emission (**14**) 1<sup>st</sup> floor

---

- field emission of *individual* MWCNTs (.2)
- CNT FED (.3, .7, .13)
- growth of CNT (.4, .6: treeCNTs, .8)
- *in situ* characterization of coiled CNT (.11)
- theory (.5, .9, .12)

# X V . 6 CNTs from tree !



**Prime Novelty:**

CNTs are grown from a botanical hydrocarbon, **Camphor**.

**Two special features:**

**1.** Three dimensional growth of CNTs on various substrates

**2.** Camphor-grown CNTs are efficient field emitters

Low turn-on field:

1 V/um

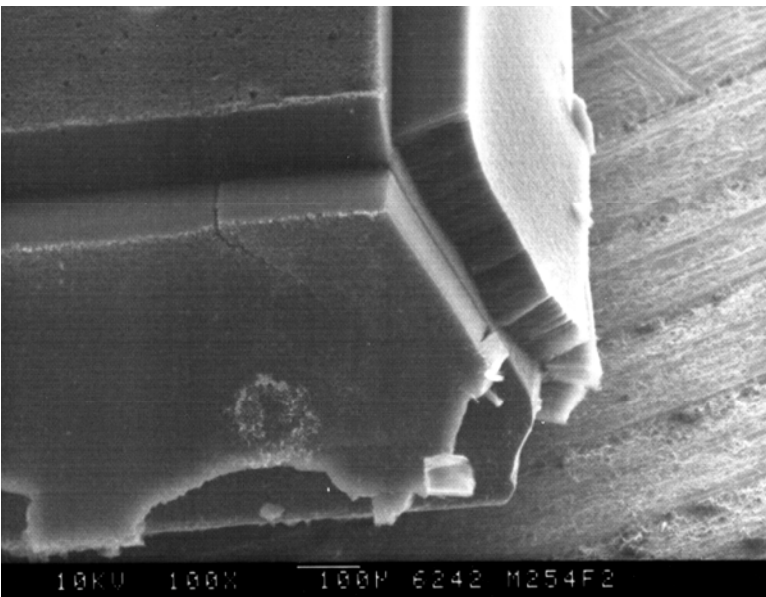
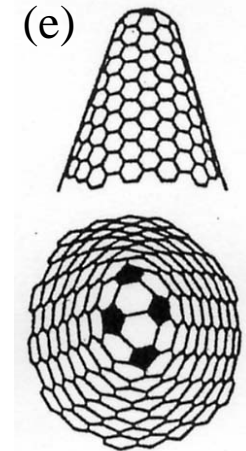
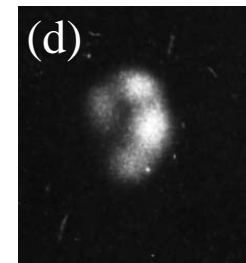
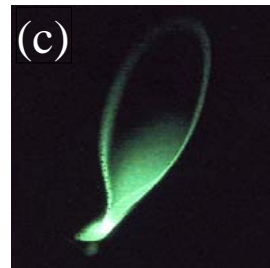
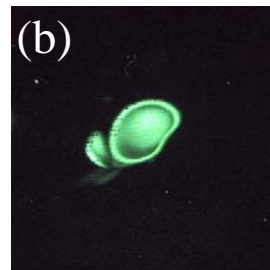
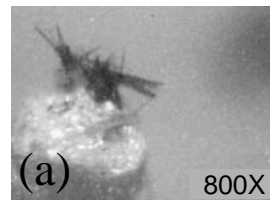
Low threshold field:

3-4 V/um

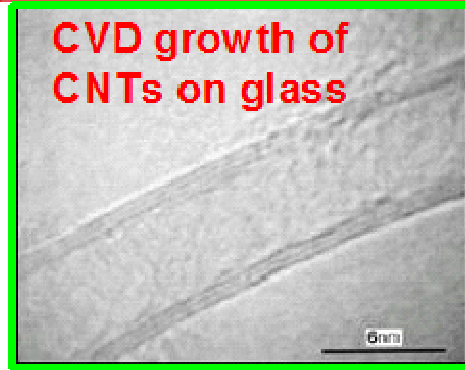
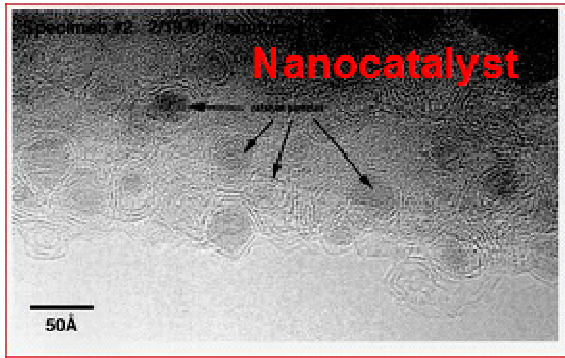
High current density:

28 mA/cm<sup>2</sup>

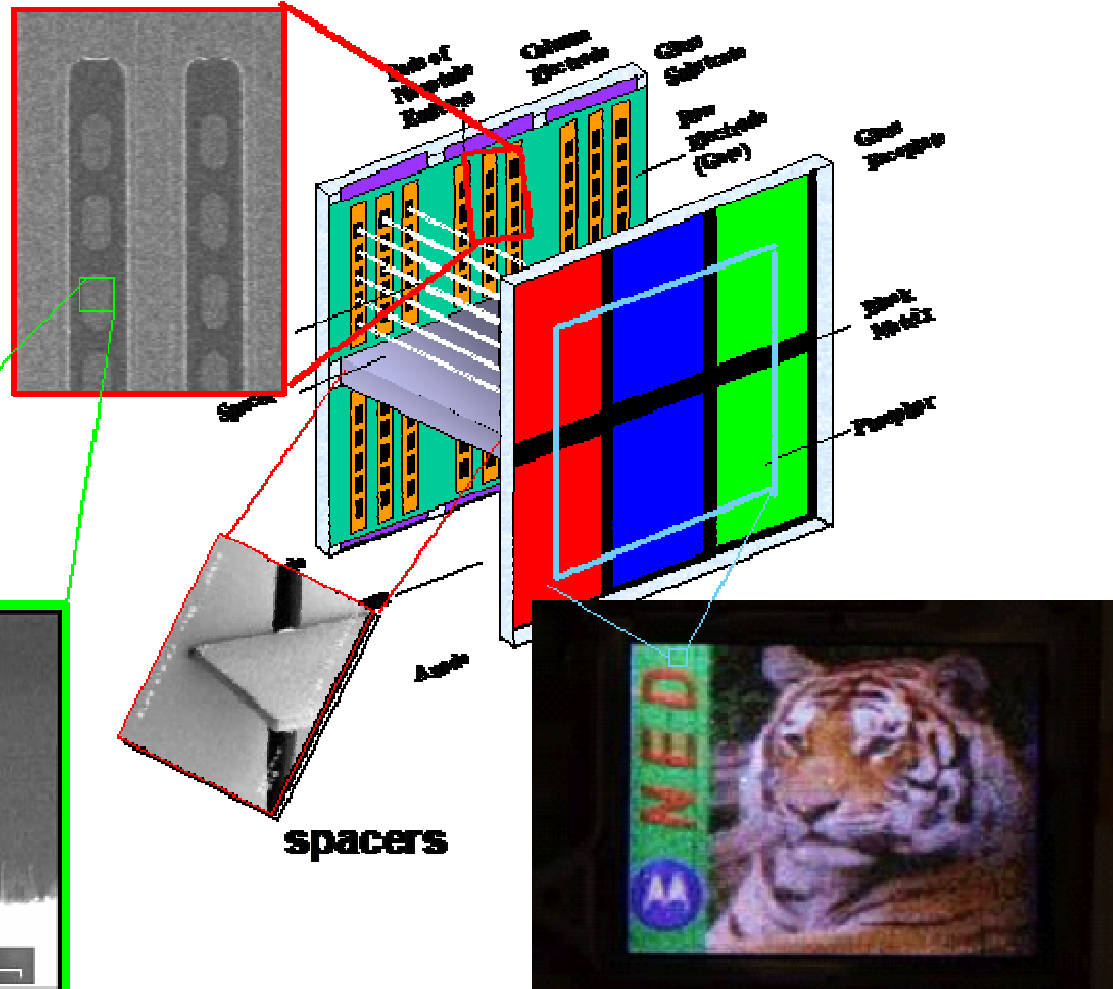
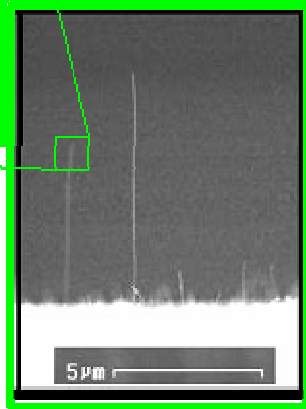
Appreciable stability



# Motorola's Nano Emissive Display (NED)



Typically 2-6 nm dia. nanotubes



Selective Nanotube Growth on Glass Substrates



Simple Field Emission Device Structure



Low Cost, High Quality Display

# Nano Emissive Displays for Large Area HDTV

## NED Prototype Performances...

4.6" NED Performances	
Peak Current Density	> 5 mA/cm <sup>2</sup> @ V <sub>F</sub> =90V 4V/μm
Switching voltage	40V
Anode voltage	6KV
Brightness	> 1500 Cd/m <sup>2</sup> in Green
Lifetime	~ 10000 hours
Uniformity	> 92%



Video Image of a 4.6" diagonal NED prototype with 726 μm pixel size which represent a piece of a 16:9 63" (1920x1080) diagonal HDTV.

## Objectives...

### Advanced HDTV with Specifications

- True HDTV (1920x1080) at Consumer Prices
- Brightness > 800 cd/m<sup>2</sup>
- Contrast Ratio 1000:1
- Enhanced Color Gamut > EBU; NTSC
- Video response time < 2ms

### High Performance

- CRT-like Color Quality
- High Brightness & Contrast
- High Grayscale Dynamic Range
- Fast Video Response
- Wide Viewing Angle
- Low Power Consumption
- Scalability in High-Definition Resolution
- Wide Temperature Range

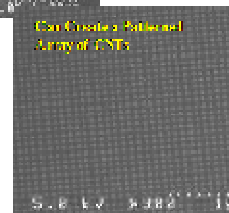
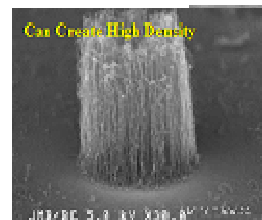
### Low Cost Planar Structure

- Simple planar Structure
- Few processing Steps
- High Manufacturing Yield
- Simple Manufacturing Process
- Low Driver Electronic Cost

## Nano Powered...

Proprietary Nano-catalyst and Chemical Vapor Deposition reactor developed and built in our Lab for growing CNTs allow:

- Selective growth
  - Controlled morphology and structure (diameter, length, number of walls)
  - Controlled density and special distribution....
- at temperature compatible with glass substrate < 550C



Manufacturing of straight and aligned CNT with a scalable process compatible with volume production and large area displays

# XVI. Optical Properties and Optoelectronics (24+1) 1<sup>st</sup> floor

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- photoluminescence studies
  - . stress induced interband transitions (.5)
  - . exciton binding energy (.16 " + 1")
  - . SWCNTs suspended in pillars (.15)
  - . red shift in PL of metallocene encapsulation (.2)
  - . DWCNTs (.21)
  - . polarized PL with <sup>13</sup>C (.22)

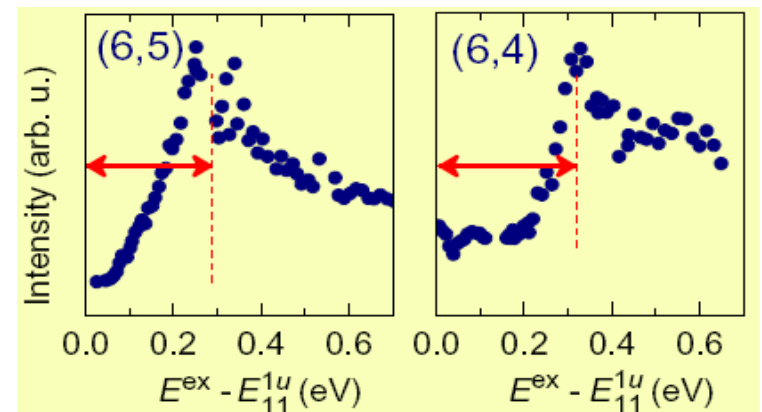
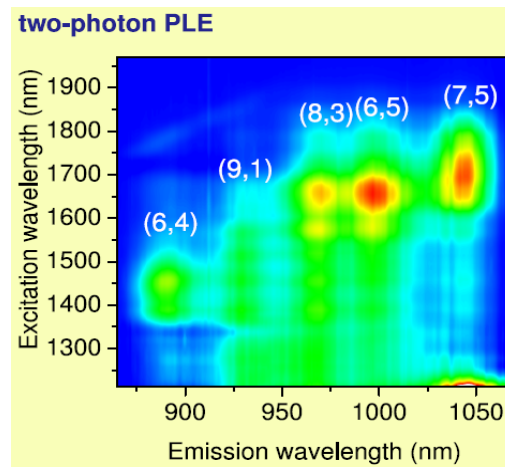
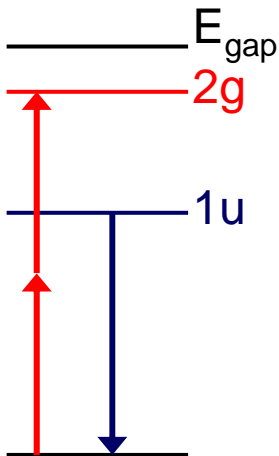


# Exciton binding energy in carbon nanotubes

XVI.16

Janina Maultzsch *et al.*

observe exciton states with different wavefunction symmetry:  
2-photon absorption ( $2g$ ) & 1-photon emission ( $1u$ )



- direct proof of excitonic nature of absorption & emission in nanotubes
- binding energies 300-400 meV

# One- and two-photon absorption in carbon nanotubes: A first-principles study

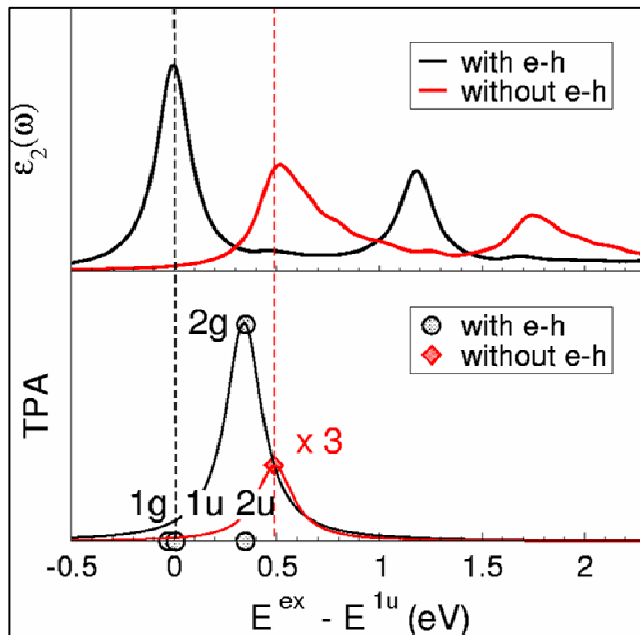
"+1"

Eric Chang, Deborah Prezzi, Alice Ruini, Elisa Molinari

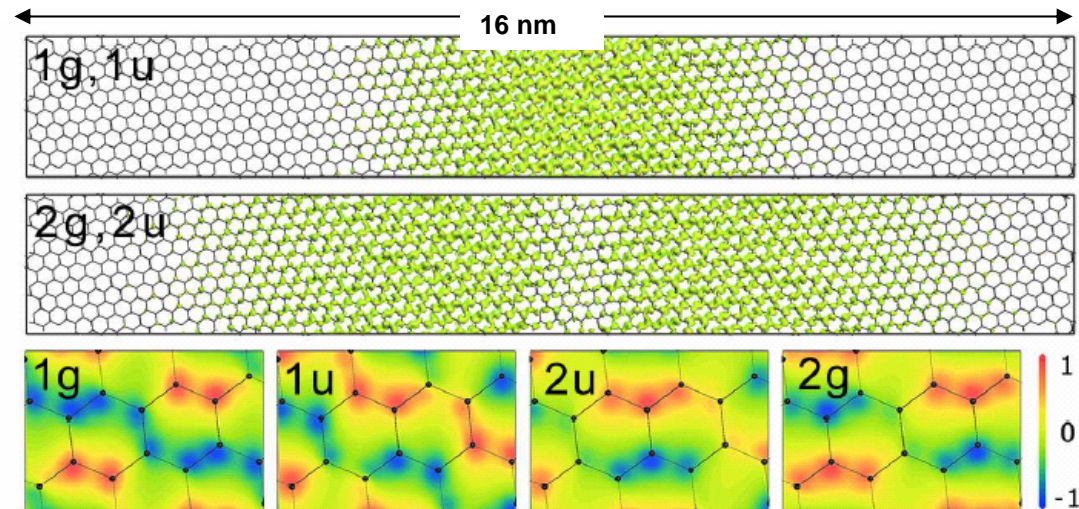
Dipartimento di Fisica, Università di Modena e Reggio Emilia and INFM-S3 National Research Center, Italy

- Bethe-Salpeter equation on a symmetrized Gaussian basis set
- (6,4) SWCNT: 152 atoms/cell & 0.7 nm diameter

## One- and two-photon optical spectra



## Exciton wavefunctions



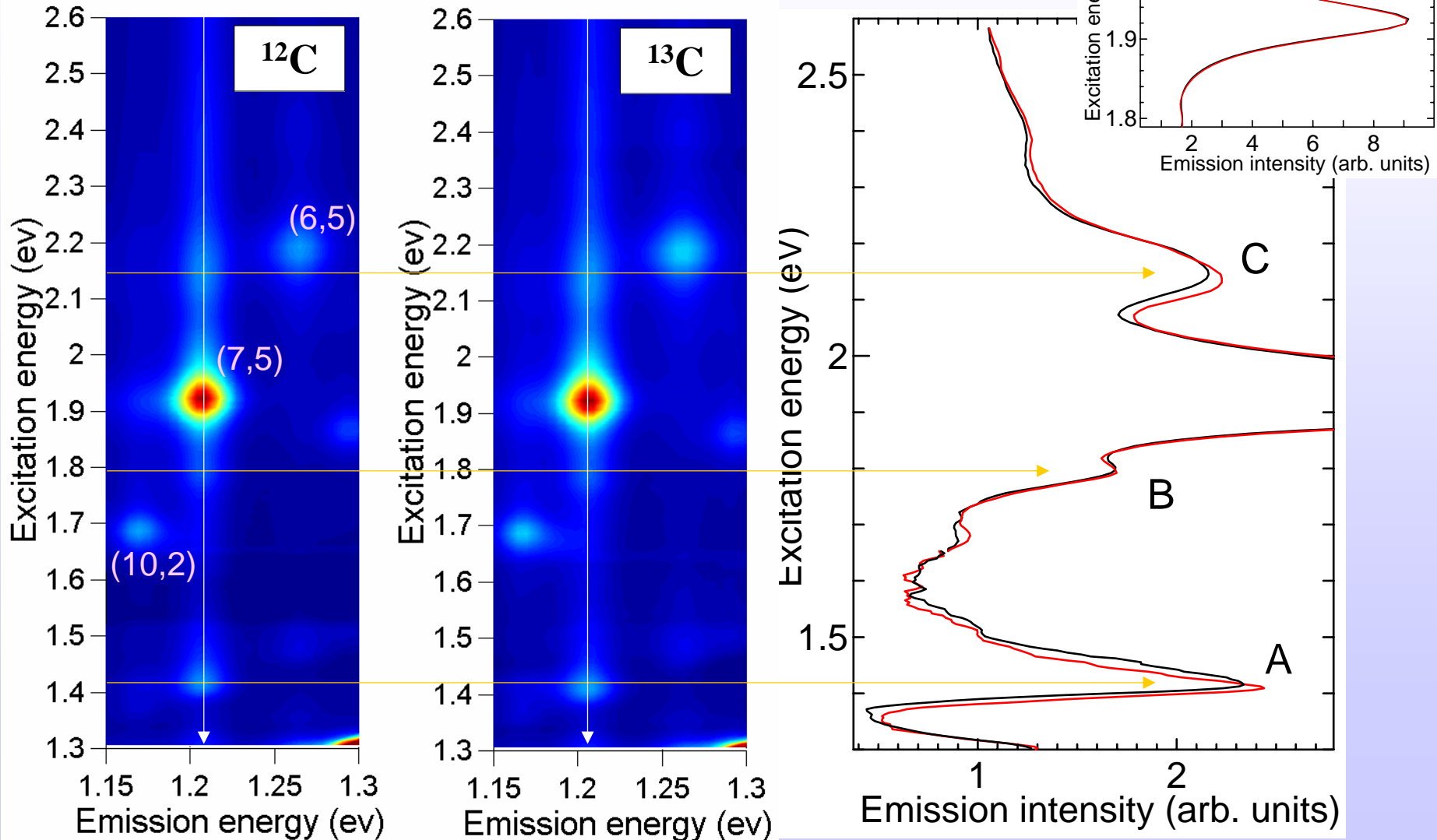
$$E_b(1g,1u) = 0.50 \text{ eV}$$

$$E_b(2g,2u) = 0.22 \text{ eV}$$

# XVI.22 Polarized-Photoluminescence Excitation Spectroscopy of Aligned Single-Walled Carbon Nanotubes by Y. Miyauchi, M. Oba, S. Chiashi, S. Maruyama

## PLE Spectra of SW<sup>13</sup>CNTs

\* PL emission at 1.208eV



# XVI. Optical Properties and Optoelectronics (24+1), 1<sup>st</sup> floor

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- photonics
  - . 3<sup>rd</sup> harmonic nonlinear optical calculations (.6)
  - . CNT-based saturable absorbers (.17, .19, .23)
- photoconduction (.8)
- lifetime of photogenerated charges
  - . slow (.10), fast (.14)
- optical transitions and phonons (.20)
- photoconduction (.8)



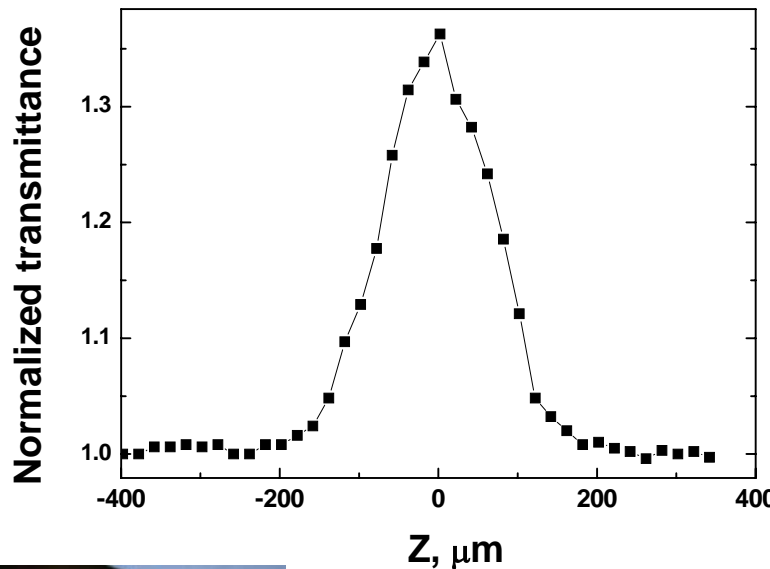
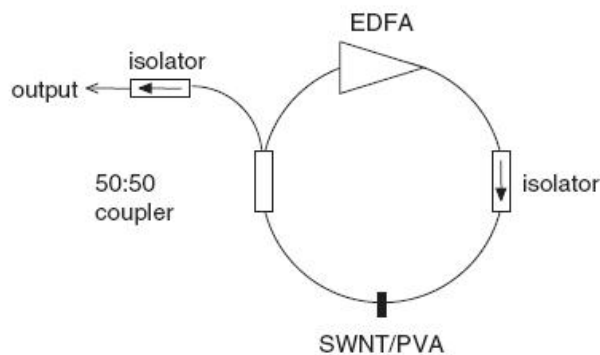
V. Scardaci, A. G. Rozhin, M. A. Reilly, M. Shaffer, A. C. Ferrari, S. Reich, I. H. White, J. Robertson, W. I. Milne

XVI

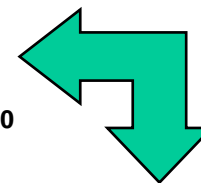
*Nanotubes: excellent materials for photonics*

.17, .19, .23

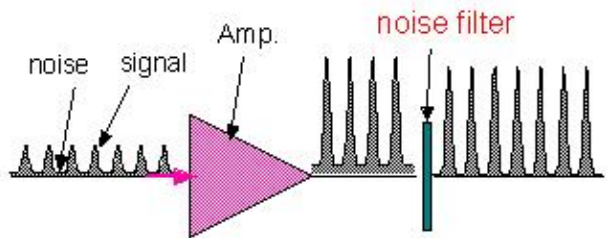
### Saturable Absorbers



PVP composites with very high optical quality

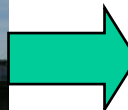


### Mode Locked Lasers



### Noise Suppression Filters

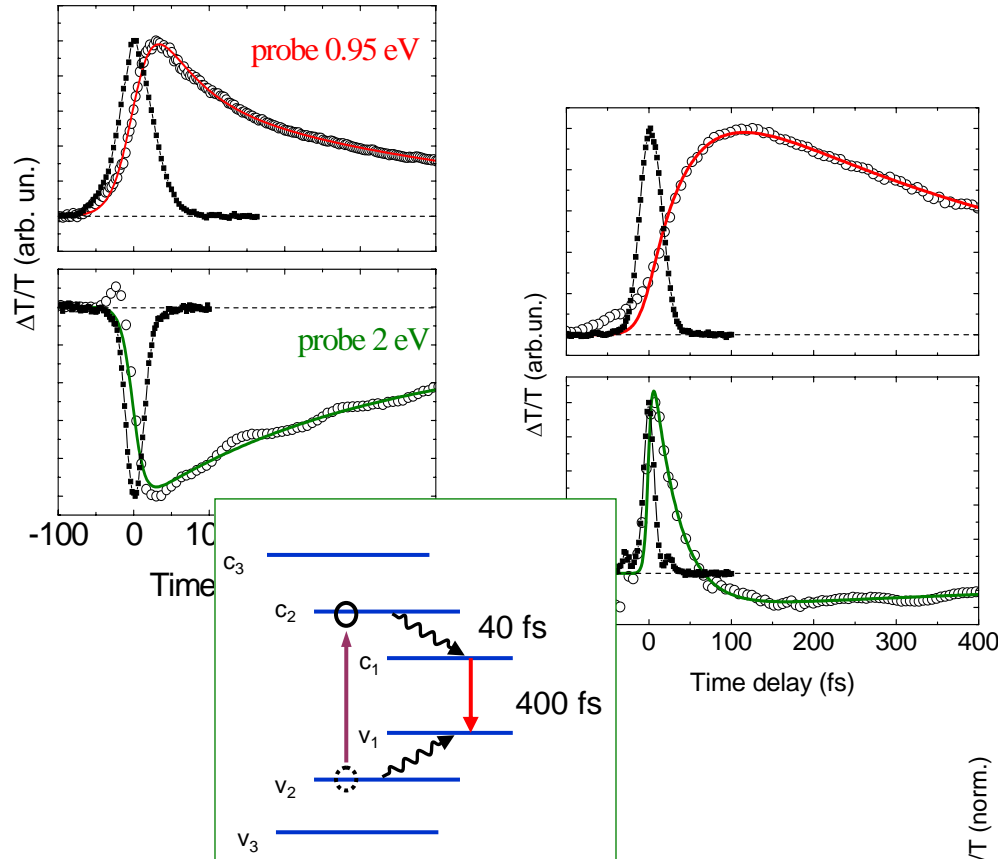
A. G. Rozhin et al.



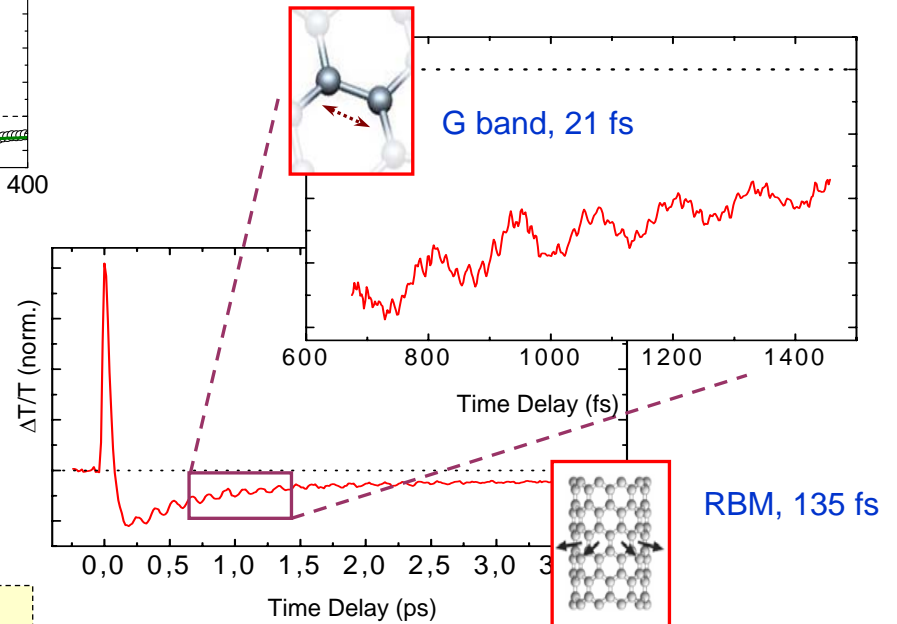
# Exciton Relaxation in Single Wall Carbon Nanotube by sub-20 fs Time Resolved Optical Spectroscopy

C. Manzoni, A. Gambetta, G. Lanzani, G. Cerullo  
 ULTRAS – INFN Dipartimento di Fisica, Politecnico, Milan (Italy)  
 E. Menna, M. Meneghetti  
 Department of Chemical Sciences, University of Padova, Italy

Poster XVI.14

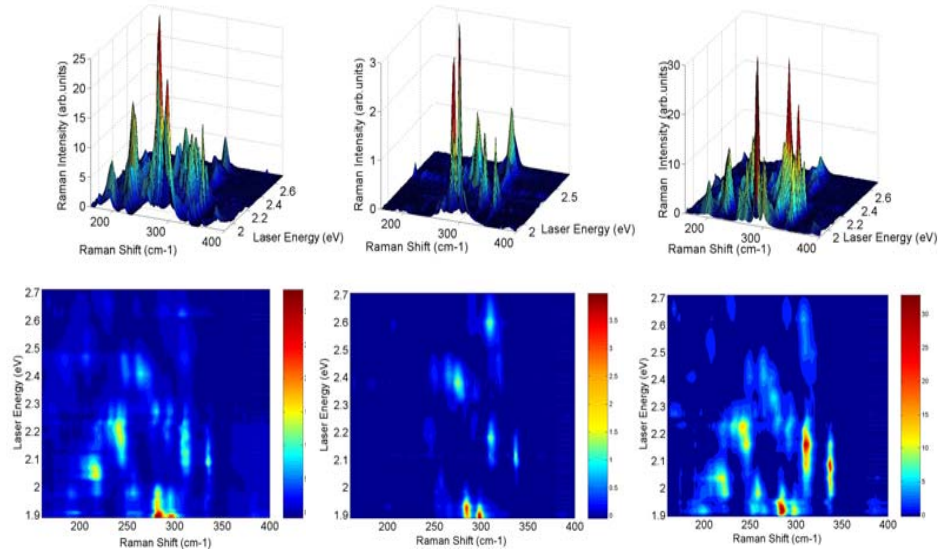


- Pump probe measurements with femtosecond pulses
- Real time observation of dynamics and oscillations



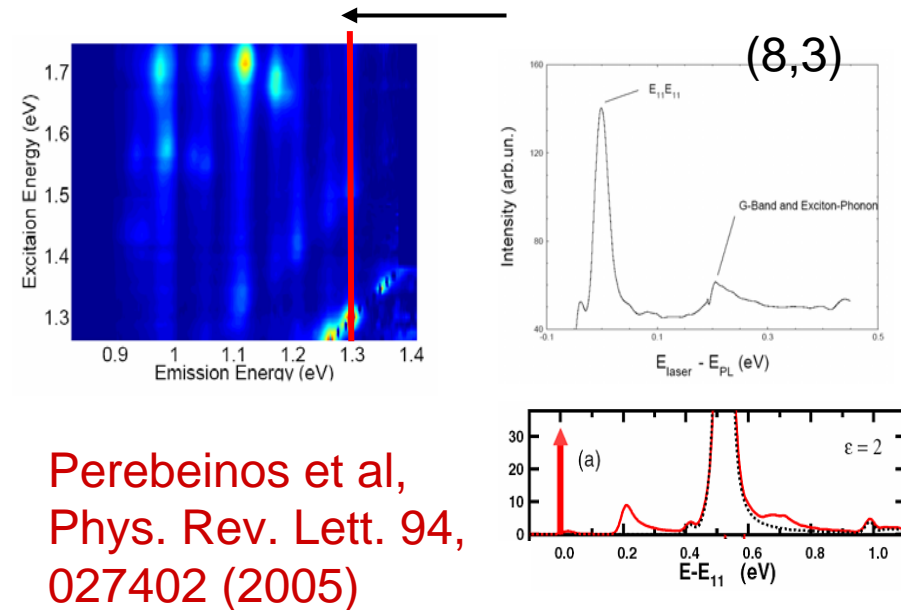
# XVI-20 Optical transitions and phonon-related processes in different samples of carbon nanotubes using resonance Raman and photoluminescence excitation spectroscopies.

## Resonant Raman spectra of CoMoCat samples



- (6,5) and (7,5) are the most abundant
- Sharp cut-off on  $dt < 0.7\text{nm}$
- Strong peak for the metallic (7,4) NT

## Photoluminescence excitation of dispersed nanotubes



Perebeinos et al,  
Phys. Rev. Lett. 94,  
027402 (2005)

Exciton-phonon coupling in the optical absorption of carbon nanotubes

# XVI. Optical Properties and Optoelectronics (24+1) 1<sup>st</sup> floor

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theory

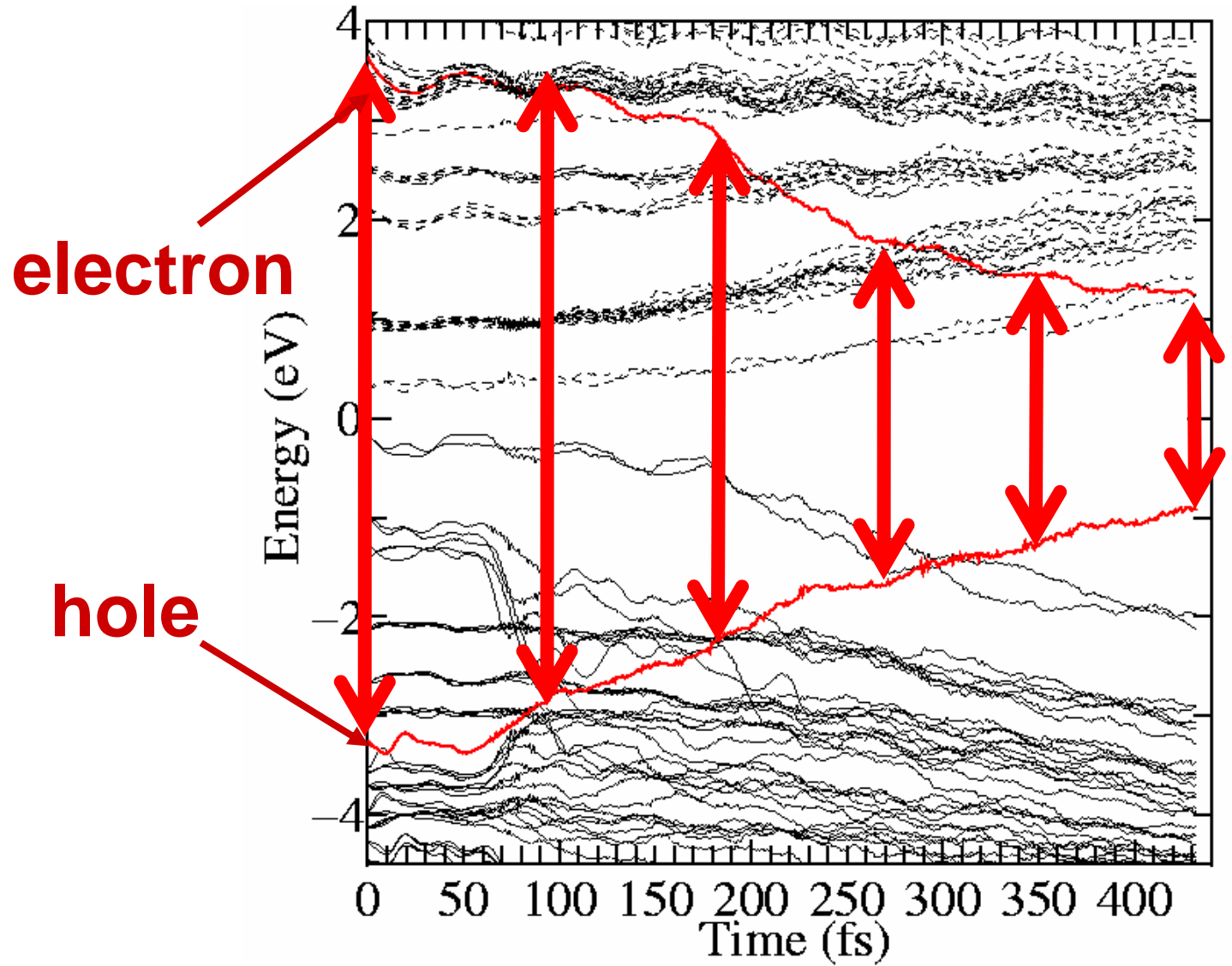
- . TDDFT for carrier decay (.1)
- . band structure calculations (.3)
- . non linear optical response (.6)
- . e-ph coupling (.12)
- . optical spectrum with E-field (.24)



# XVI.1

TDDFT-MD simulation for ultra-fast carrier decay in nanotubes: Dependence on lattice temperature

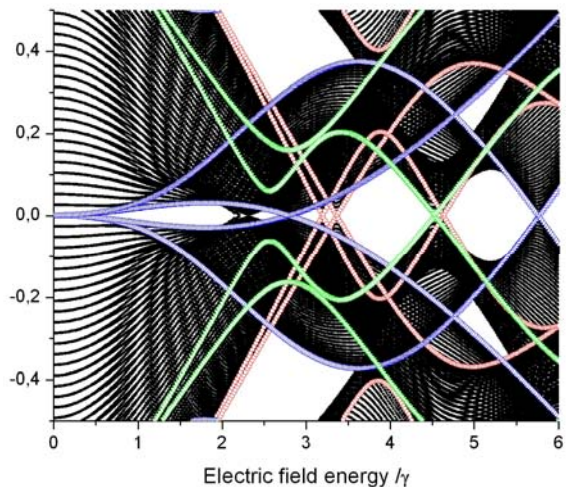
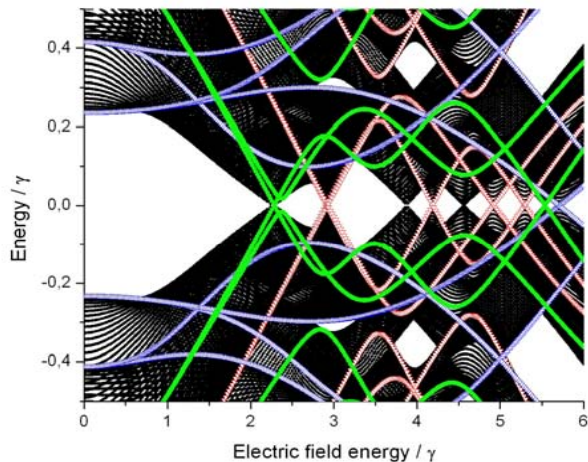
Yoshiyuki Miyamoto, Angel Rubio, and David Tománek



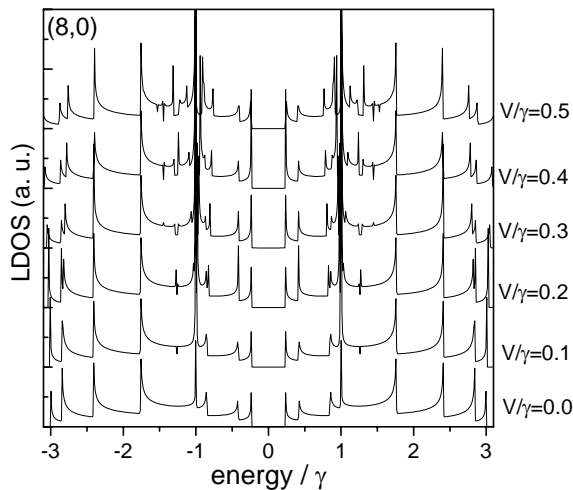
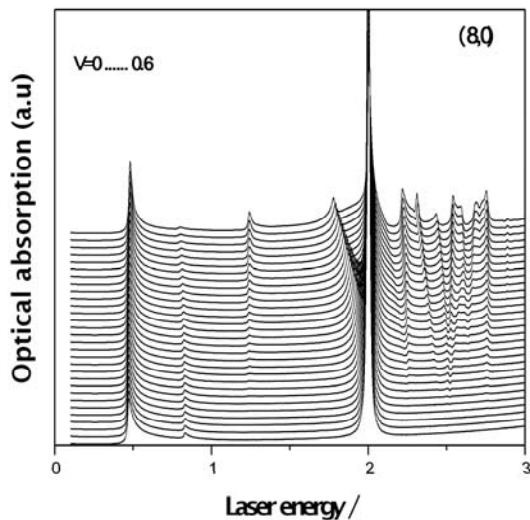
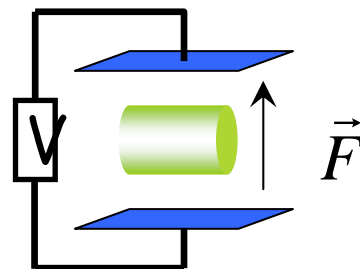
# POSTER XVI 24

## Optical properties on carbon nanotubes under external fields

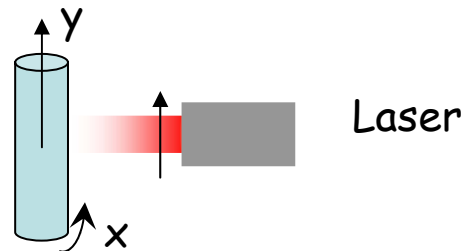
M. Pacheco\*, C. G. Rocha†, Latgé†, Z. Barticevic\*



Energy spectra for ZZ CNT as a function of an Electric field



Optical absorption and DOS for different EF values



# XVII. Transport in Complex Nanostructures (4), 2<sup>nd</sup> floor

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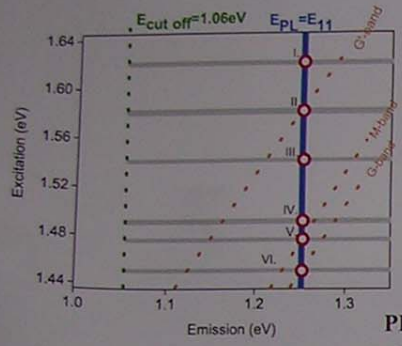
- molecular mechanics (.1T)
- e-transport of CNTs embedded in polymer macrotubes (.2)
- STM response of a Luttinger liquid (w/ Kondo) (.3T) [**the only on!**]
- *chemical* diffusion through flower-like bundle of manganese oxide nanofibers (.4)

# XVIII. Electron-Phonon Coupling in Complex Nanostructures (2), *2<sup>nd</sup> floor*

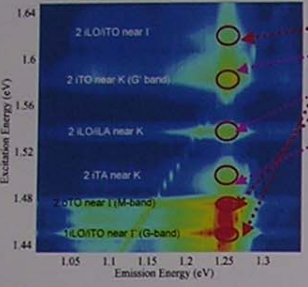
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- Family pattern in electron-phonon matrix elements and relaxation time in carbon nanotubes (.1)
- Experimental electron phonon coupling in graphite and nanotubes (.2)

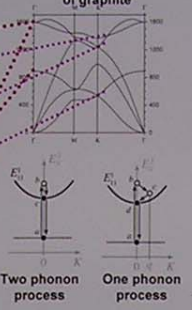
Relaxation process in semiconducting tubes



PL spectra of (6,5) tubes  
S. G. Chou, et al PRL 94, 127402 (2005)

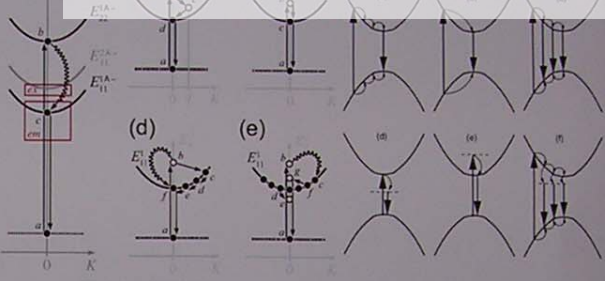


Phonon dispersion relations of graphite

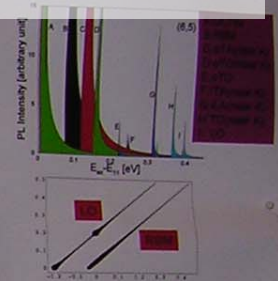


Two phonon process  
One phonon process

XVII. 12 + XVIII. 1



Exciton picture

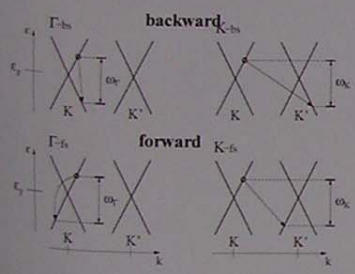


Band-band picture

S. G. Chou, et al PRL 94, 127402 (2005)

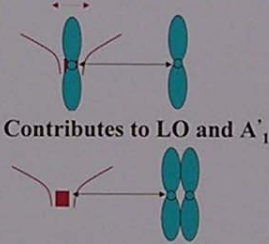
J. Jiang, et al PRB 71, 045417 (2005)

Inelastic scattering in metallic tubes: transport properties



Forward and backward scattering processes

mode	Forward		Backward	
	$g$ (eV/Å)	$\tau$ (ps)	$g$ (eV/Å)	$\tau$ (ps)
LA	0	0	0	0
TW	0	0	0.163	6.944
RBM	0.567	3.300	2706.00	0
$\sigma$ TO	0	0	1.119	12.391
iTO	8.088	0.434	355.88	0
LO	0	0	6.805	0.757
$E_2'(1)$	0	0	0	0
$E_2'(2)$	0	0	2.959	1.072
$A_2'$	0.177	0	0	0
$E_1'(1)$	11.031	0.1926	157.93	0
$E_1'(2)$	0	0	11.658	0.159
$A_1'$	0	0	9.828	0.281

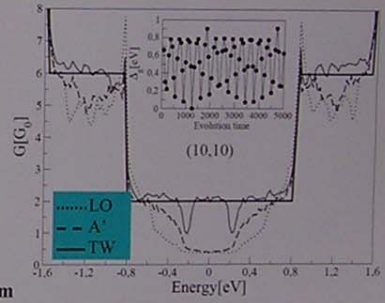


Contributes to LO and A'1

Contributes to E'1

Backscattering mean free path: 67 nm

Jiang et al., unpublished



"Baboo dancing effect"

$$D_E(t) = \frac{1}{t} \langle X(t) - X(0) \rangle^2 >_E$$

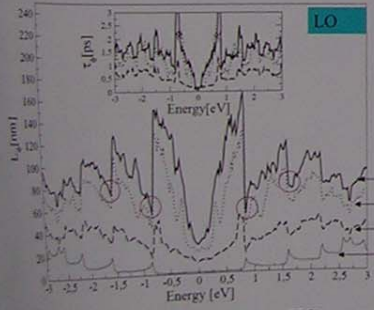
$X(t)$ : position operator

$$G(E) = \frac{2e^2}{L} \lim_{t \rightarrow \infty} \text{Tr}[\delta(E - H) D_E(t)]$$

S. Roche et al. unpublished.

This work is recently submitted by S. Roche, J. Jiang, F. Triozon, R. Saito

Relaxation time by Fermi Golden rule



L decreases much at vHS

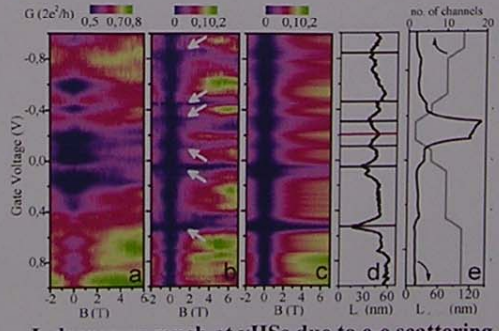
S. Roche et al. unpublished.

$N_{\perp}(E)$ : number of conducting channel

$$G(E, t) = \frac{2e^2}{L} \text{Tr}[\delta(E - H) D_E(t)]$$

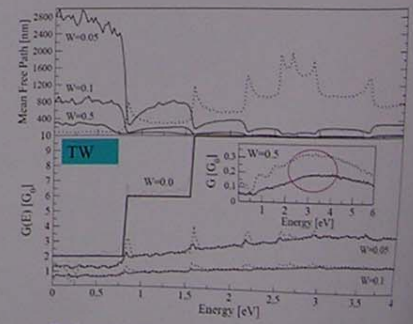
$$G(E, t) = \frac{2e^2}{h} \frac{N_{\perp}(E) L_{\phi}(E)}{L(E, t)}$$

$A_0$ : Phonon amplitude  
At T=300K



L decreases much at vHS due to e-e scattering

B. Stojetz, et al PRL 94, 186802 (2005)



Delocalization by inelastic scattering

S. Roche et al. unpublished.

# Family patterns in the electron-phonon matrix elements and relaxation time in carbon nanotubes

J. Jiang<sup>1</sup>, R. Saito<sup>1</sup>, Y. Oyama<sup>1</sup>, K. Sato<sup>1</sup>, A. Grueis<sup>2</sup>, S. G. Chou<sup>3</sup>, Ge. G. Samsonidze<sup>3</sup>, A. Jorio<sup>4</sup>,  
F. Triozon<sup>5</sup>, S. Roche<sup>5</sup>, G. Dresselhaus<sup>3</sup>, M. S. Dresselhaus<sup>3</sup>

<sup>1</sup>Tohoku University and CREST JST, Sendai Japan, <sup>2</sup>IFW, Dresden, German

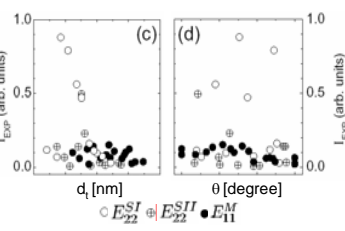
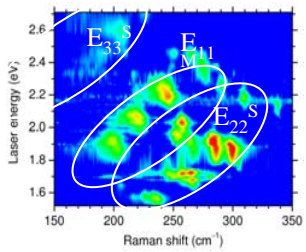
<sup>3</sup>MIT, Cambridge, MA USA, <sup>4</sup>Univ. Fed. Minas Gerais, MG, Brazil, <sup>5</sup>CEA/DSM/DRFMC/SPSMS, France

E-mail : [jiang@flex.phys.tohoku.ac.jp](mailto:jiang@flex.phys.tohoku.ac.jp) Web: <http://flex.phys.tohoku.ac.jp>



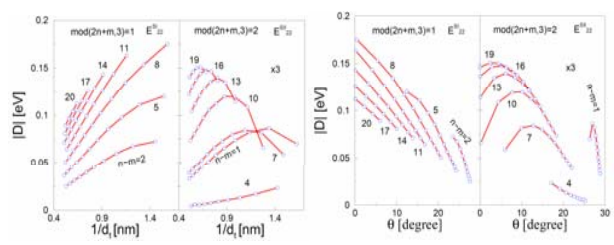
## Family patterns and quantum interference in RBM Raman intensity

Measured RBM Raman intensity



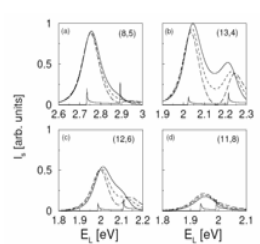
Jorio et al., 71, 075401, 2005

Calculated electron-phonon matrix elements.

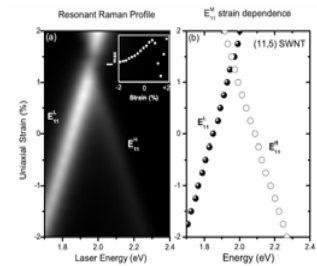


Both gives same family patterns

Quantum interference predicted by theory



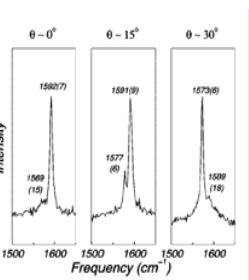
Quantum interference observed by experiment



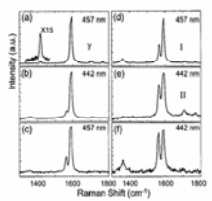
J. Jiang et al, 71, 205420 (2005) A. G. Souza Filho et al, unpublished

## Family patterns in Raman intensity of G band

Measured G-band Raman intensity

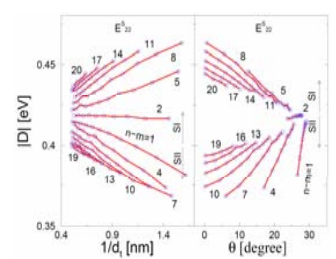


R. Saito et al, Phys. Rev. B 64, 085312 (2001)



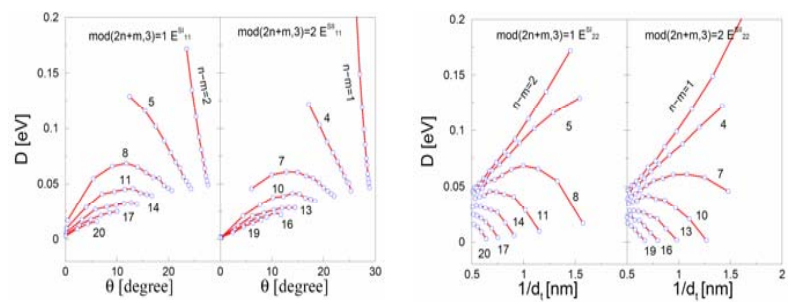
Z. Yu et al., J. Phys. Chem. B 105, 1123 (2001)

Calculated electron-phonon matrix elements for LO mode



Family patterns in the matrix elements explain well the measurements

Calculated electron-phonon matrix elements for TO mode



# Experimental

## Electron-Phonon-Coupling in Graphite and Nanotubes

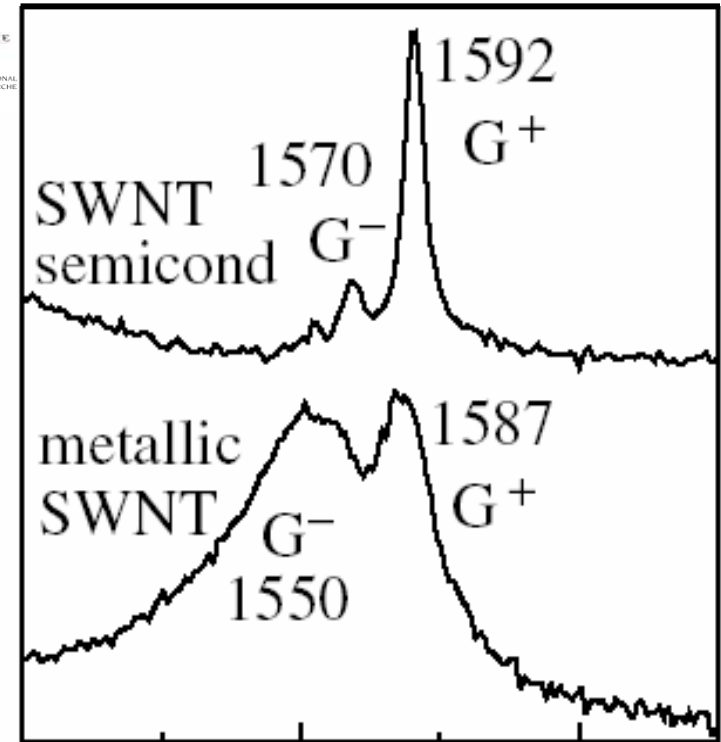
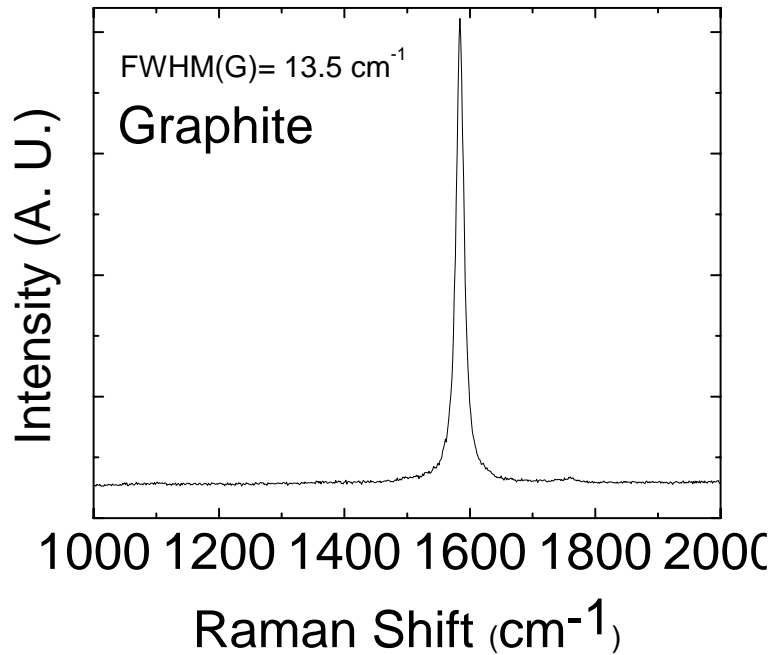
A. C. Ferrari, M. Lazzeri, S. Piscanec, F. Mauri, J. Robertson



UNIVERSITY OF  
CAMBRIDGE



$$FWHM(G) \propto EPC^2(\Gamma)$$



$$FWHM(G^-) \propto \frac{EPC^2(\Gamma)}{d}$$

- Kohn anomaly → down shift
- EPC → broader peak

**NO PLASMON FANO RESONANCE**

# wish list (... for transport)

---

- transport with non equilibrium e+ph
- FM contacts: spin injection
- phase coherence length and e-mean free path in (2+)WCNTs
- limits for Luttinger / non-Luttinger
- superconducting contacts
- ...

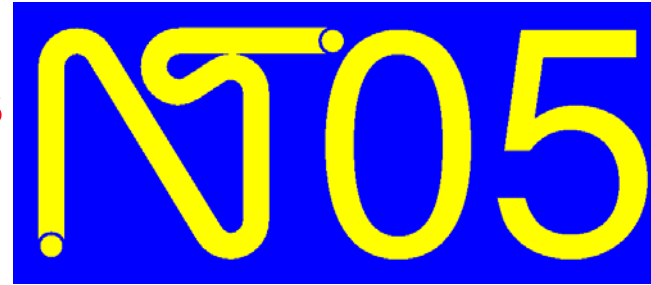


**NT05: Sixth International Conference on the  
Science and Application of Nanotubes**

***Göteborg, Sweden***

***June 26 - July 1, 2005***

**<http://nanotube.msu.edu/nt05/>**



**B.5 Yoshiyuki Miyamoto Friday, July 1**



**Poster session B.5**

**47 presentations  
(Third floor)**

**Poster chair**

**Yoshiyuki Miyamoto, NEC**



Poster XIX.1-10

Challenge to nanotube electronic devices

Poster XX.1-7

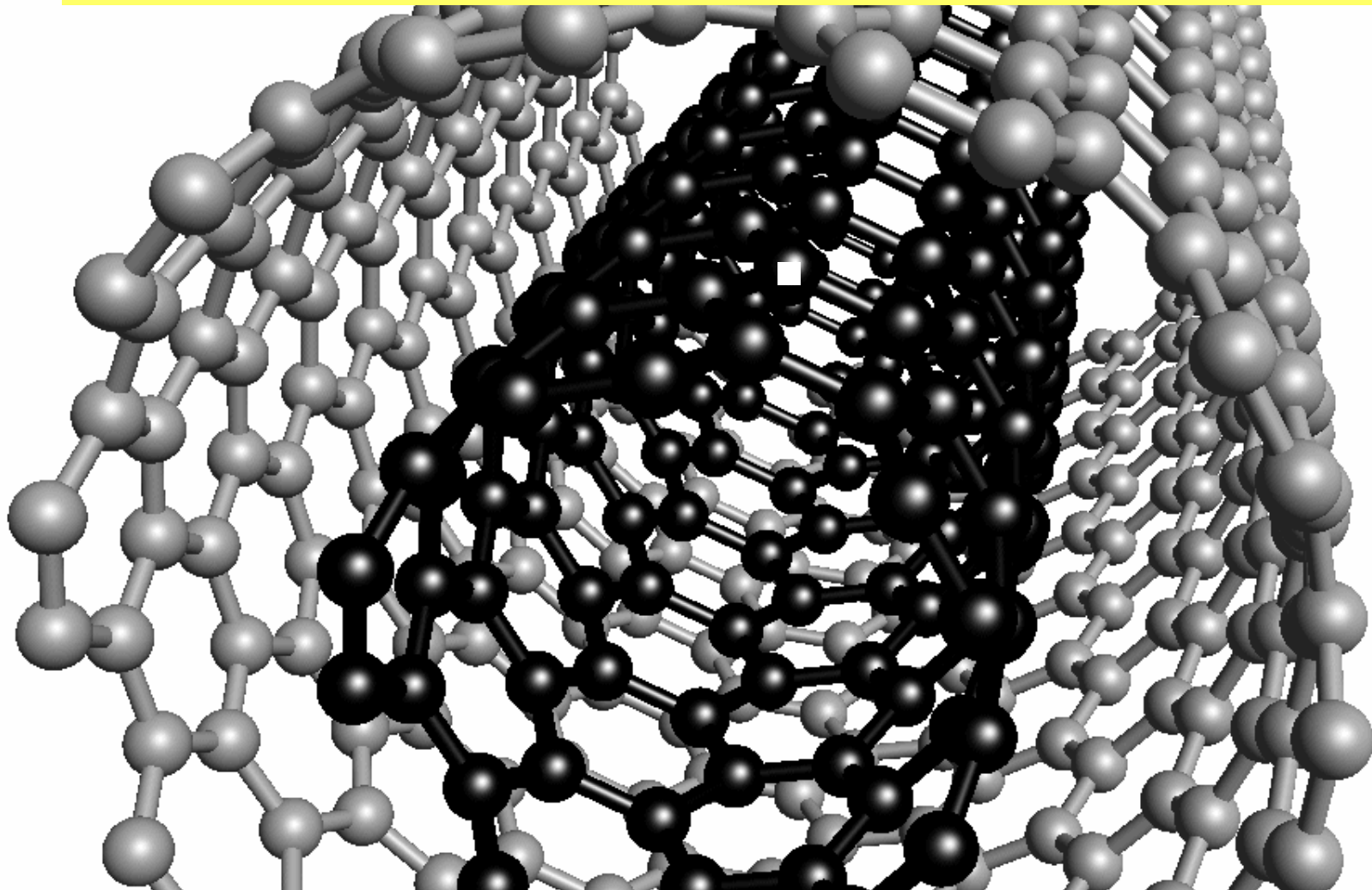
Magnetic property of nanotubes

Poster XXI.2-31

Others (the most challenging part for chairing)

**Every Poster seems to be quite new for me.  
Many new approaches are going  
otherwise  
the poster chair doesn't know anything about nanotubes.**

**Poster XIX.1-10**  
**Challenge to nanotube electronic devices**  
**(Transistors)**



**XIX.1 Field emitting transistor**

**XIX.2, XIX.6 e-irradiated Metal-semiconductor transition in FET**

**Chirality change? Maybe not?**

**XIX.3, XIX.10 Stable n-type FET (XIX.3 Alkali atoms are inside, XIX.10 PMMA passivation)**

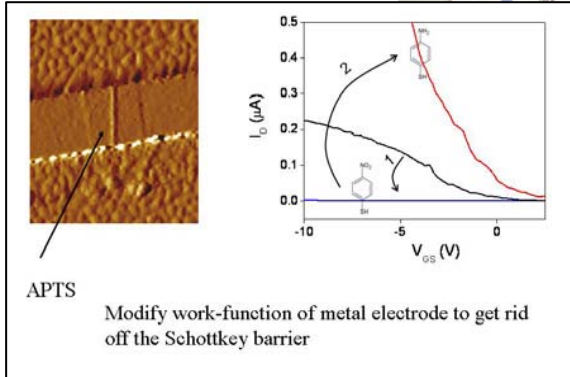
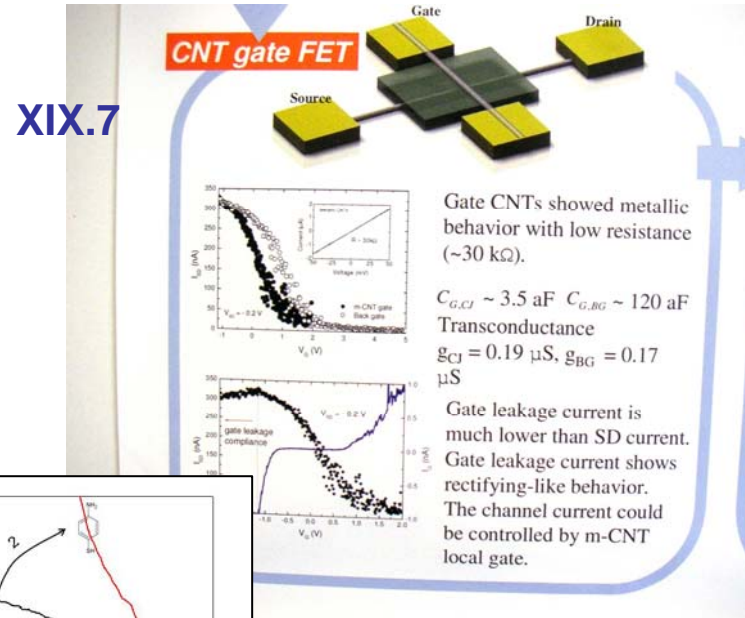
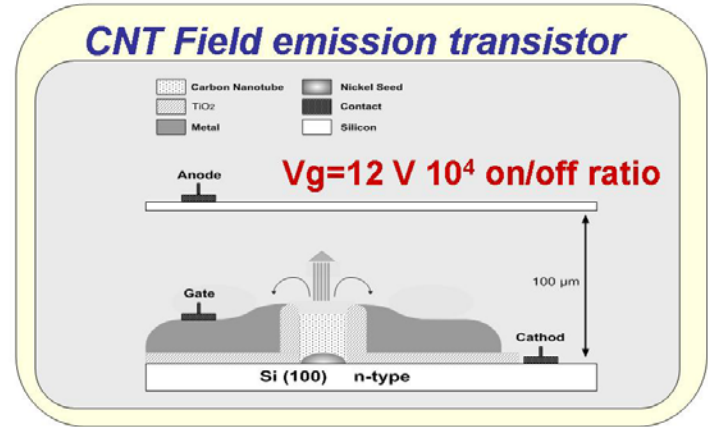
**XIX.4, XIX.5 FET as biochemical sensors**

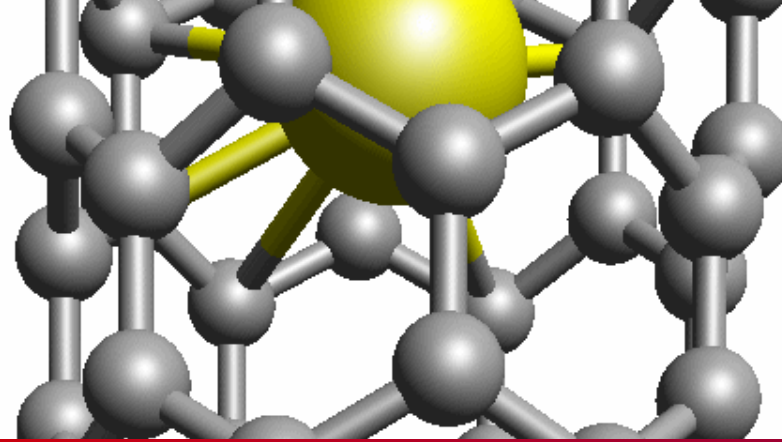
**XIX.7 CNT-gated CNT-FET! (World smallest CNT transistor!)**

**XIX.8 Standing CNTs on magnetic semiconductor substrate (spintronics)**

**XIX.9 Barrier control with use of **XIX.9 chromophore functionalization****

**XXI.28 Contact Resistance of CNT Coated Surfaces**





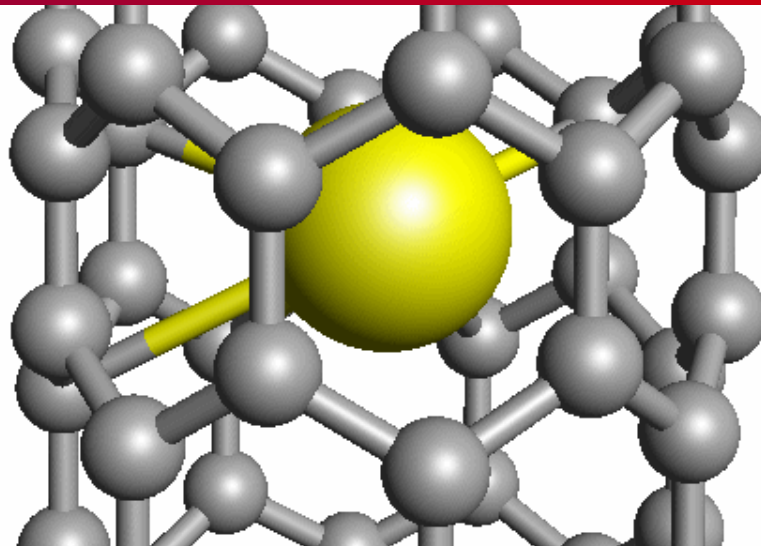
Poster XX.1-7

Magnetic property of nanotubes

New recording media

Encapsulation of magnetic metals

Influence of Magnetic field



**XX.1 Realization of  $\alpha$ Fe inside CNT**  
**-> strong magnetization!**

**XX.2 CNT under magnetic field**  
**(Theory)**

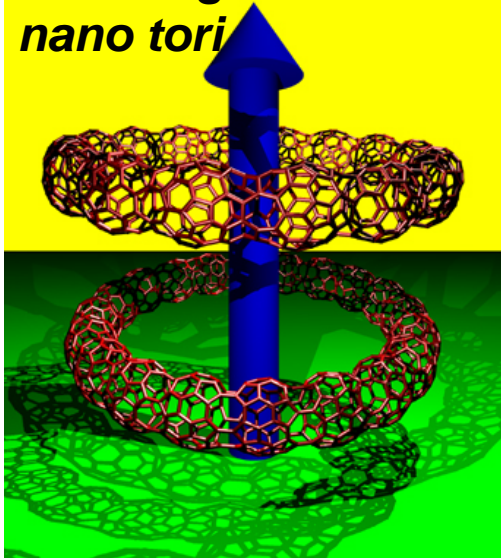
**XX.3 M@SWNTs targeting spintronics**

**XX.4 under magnetic field and  $V_g$  control**

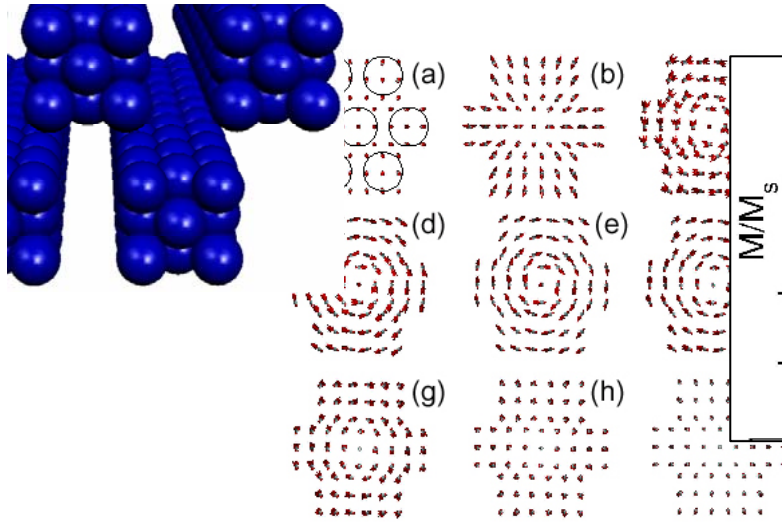
**-> weak localization, AAS oscillations**

**XX.5 aligned particle in top/end of CNT targeting high-density memory**

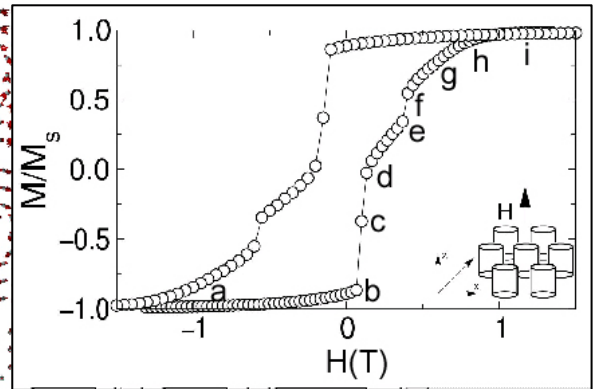
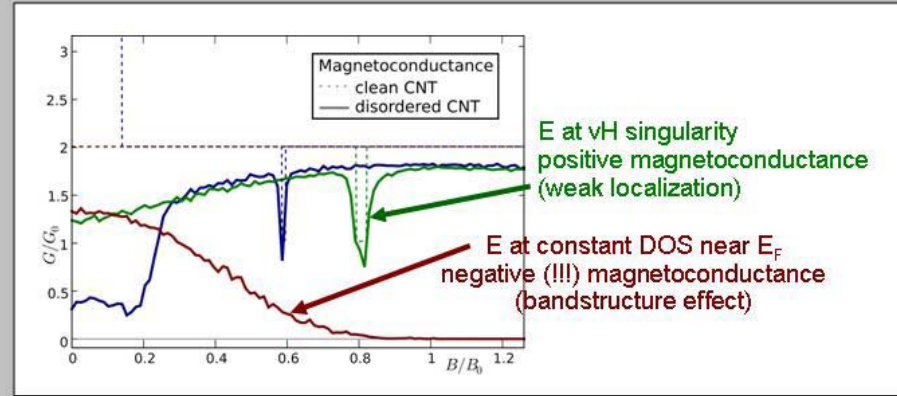
**XX.6 ring current in nano tori**



**XX.7 Magnetization Studies of Fe NWs**



**XX.2**







# Poster XXI.2-31 Others!

- **Growth again (experiment & theory)**
- **Fabrication/Process**
- **Characterization (experiment/theory)**
- **Other applications (Environmental, Bio, Actuator)**
- **Review**

# Growth (experiment)

XXI.18 withdrawn

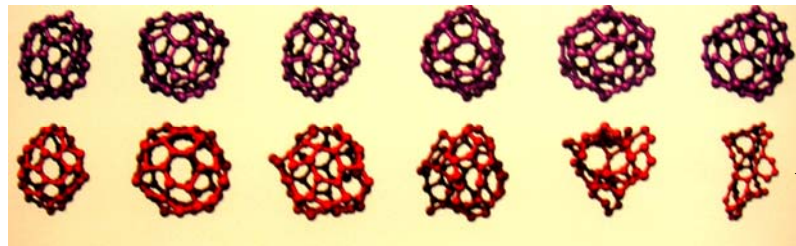
XXI.23 withdrawn

# Growth (Theory/Simulation)

XXI.4 growth on (100)(111) surface

XXI.9 Influence of monoatomic steps of nickel during the nucleation of C-SWNTs

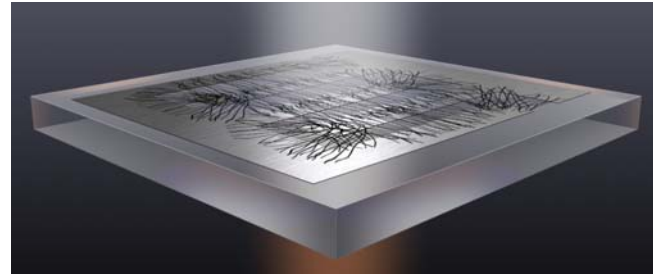
XXI.15 MD Test of heat bath->NG!: for each atom, Good!: for the system



Over melting with heat bath for each atom

# Fabrication/processes

**XXI.3** Sort metallic tube by high-frequency field: for any diameters!



**XXI.6** Direct structuring of SWNT free standing thin films

**XXI.10** MD-examination for successful substitution of B/N as 30%/40%, sharp difference of diffusion barrier B(0.1eV)/N(1.1eV)

**XXI.12** Location Control of CNT Etched pattern on SiO<sub>2</sub> and growth

**XXI.17** LPCVD Apply E in order to separate SWNT, MWNT, M-particle,  $\alpha$ -C from product.

**XXI.26** H-impact induced structural change -> electronic structure change

# Characterization (Experiment)

**XXI.8** First-time measurement of micro-X-ray diffraction : Nature of catalytic particles from root to top of CNT.

**XXI.14** fullerene-like structures' metal derivatives  
Structural magnetic properties by Mass, EPR, NMR, X-ray, Raman...

**XXI.19**  $^{13}\text{C}$  NMR study of alkali-CNT  $N(E_F)$  and preferential site

**XXI.20** Electrostatics of individual SWNTs investigated by EFM

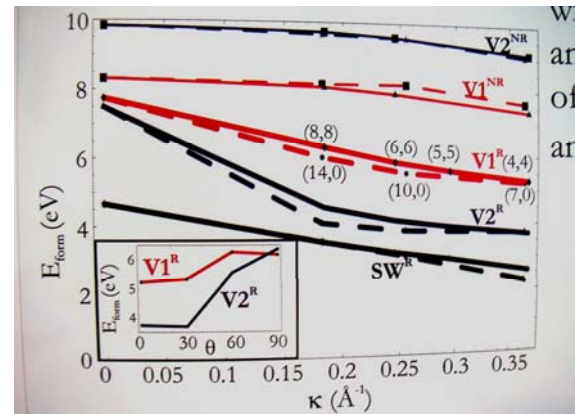
**XXI.22** SWNT Light-Assisted Oxidation -> appeared in change of FL  
Light-induced selective burning/removal of CNT with  $\text{H}_2\text{O}_2$

**XXI.27** Determination of Nanotube Density by Gradient Sedimentation  
Mass/Volume wrt bundle size vs. geometrical simple model.

**XXI.29** Mechanisms of electromigration of inner Fe atoms is addressed from cross-sectional structure by TEM

# Characterization (Theory)

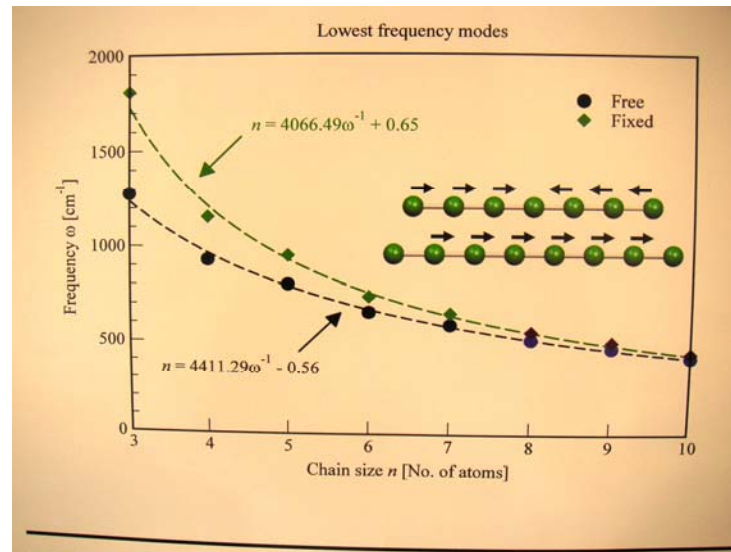
## XXI.7 Curvature assisted defects in nanotubes



## XXI.24 Low energy instabilities of small-radius zig-zag nanotubes

e-e Coulomb-repulsion vs e-phonon-mediated e-e attraction

## XXI.31 vibrational and electronic structure of 1D C-chains (even/odd # of C atoms)



# Other applications

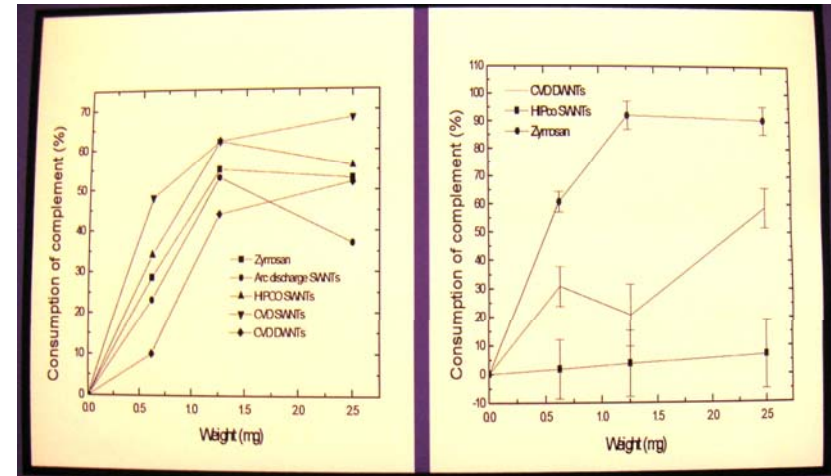
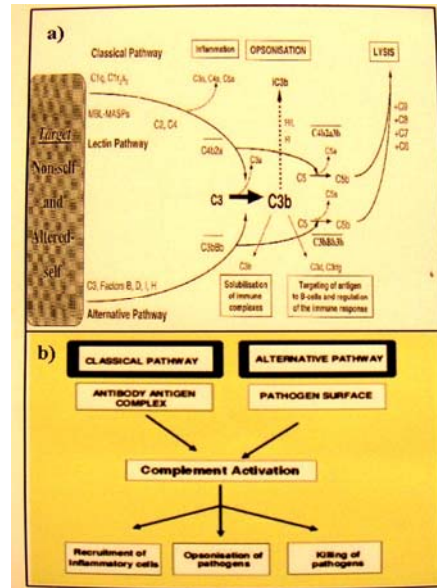
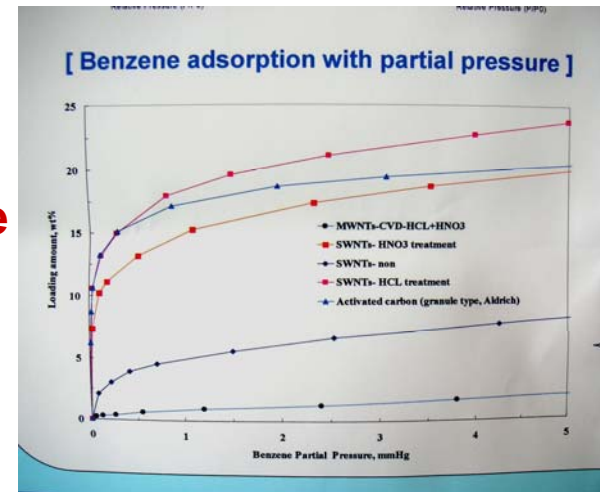
**XXI.11** The Adsorption of Hazardous Organic Compounds **SWNT shows better performance than activated carbon**

**XXI.13** Novel actuator with SWNT (Theory)

**Charge-induced forces on  $10^{13}$  aligned SWNTS!** (Theoretical-patent pended)

**XXI.21**

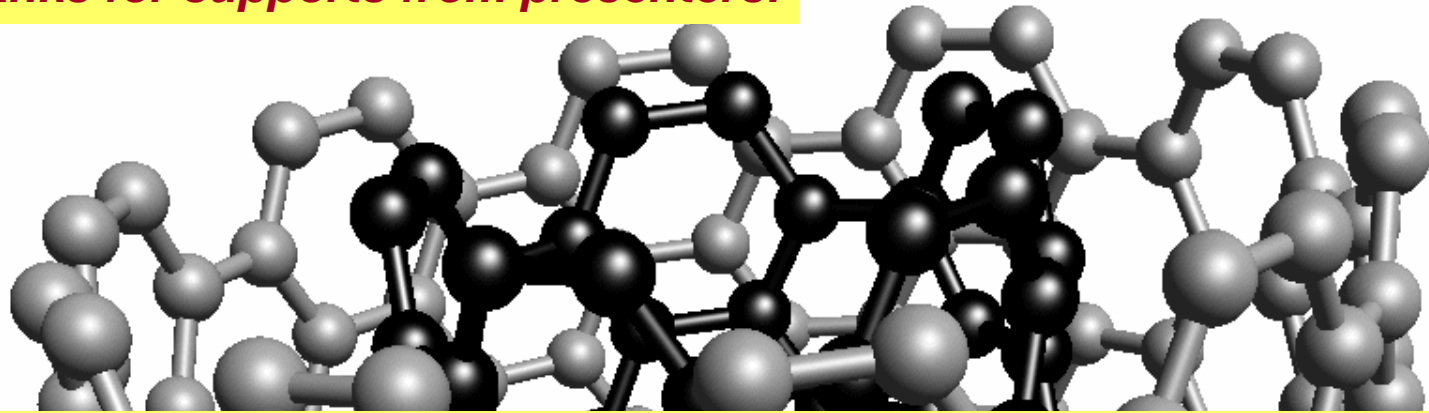
**'We report for the first time that carbon nanotubes activate human complement via both classical and alternative pathways.'**



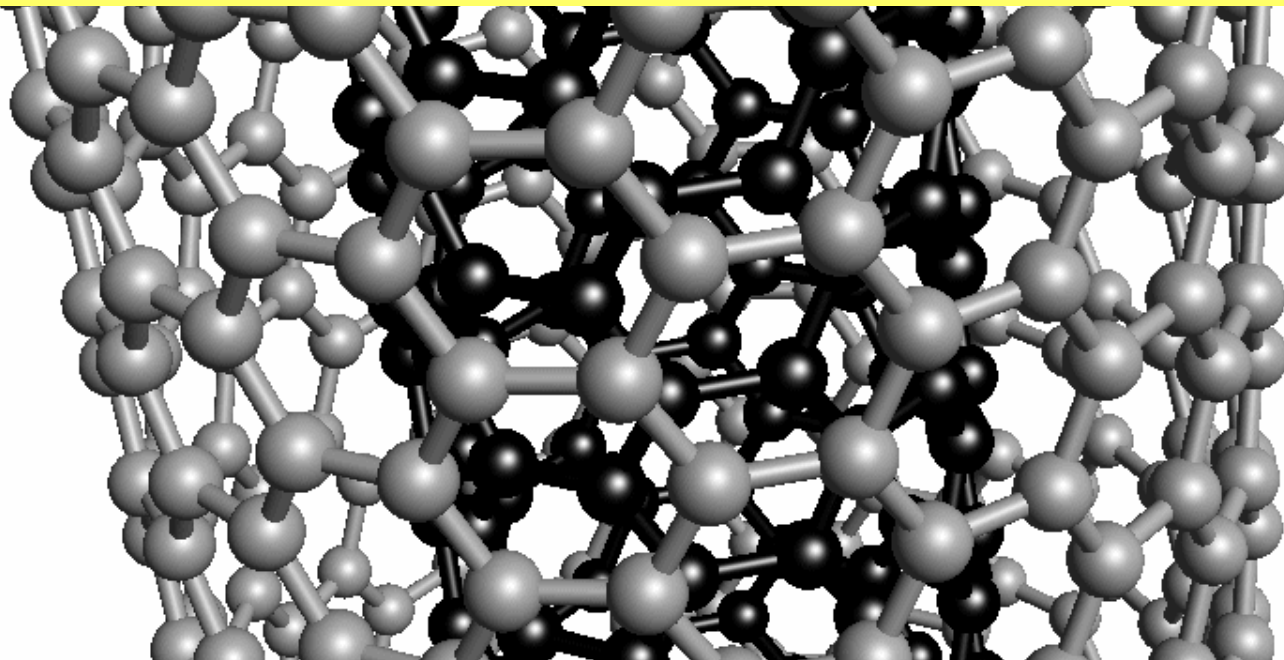
# Review

XXI.2 withdrawn

*Thanks for supports from presenters!*



**Good fortune often comes from  
remaining things!**





**Poster XIX.1** *Carbon Nano-tubes for the fabrication of high on-off ratio field-emission transistors* **Surrounding gate on cathode tube- $\rightarrow V_g=12\text{ V } 10^4$  on/off ratio**

Y. Abdi, J. Koohsorkhi, A. Miri, and S. Mohajerzadeh

**Poster XIX.2** *Metal-semiconductor transition in single-wall carbon nanotubes induced by low energy electron irradiation*

A. Vijayaraghavan, K. Kanzaki, S. Suzuki, Y. Kobayashi, S. Kar, P. M. Ajayan

**Poster XIX.3** *Air-stable n-type single-walled carbon nanotubes with alkali-metal encapsulation performed by plasma ion irradiation*

T. Izumida, T. Hirata, R. Hatakeyama, Y. Neo, H. Mimura, K. Omote, and Y. Kasama

**Poster XIX.4** *... on Carbon Nanotubes*

**Bio-applications!!**

**Poster XIX.5** *...ors*  
Brian Hunt, ...vills

**Poster XIX.6** *Conductivity control of single-walled carbon nanotubes by electron beam exposure*

K.Kanzaki, A.Vijayaraghavan, S.Suzuki, Y.Kobayashi, H.Inokawa, Y.Ono

**Poster XIX.7 Fabricatin of Crossed Semiconducting and Metallic Nanotubes: CNT-gated CNT-FET**

D.S. Lee, J. Svensson, S.W. Lee, Y.W. Park, E.E.B. Campbell

**Poster XIX.8 1D-Carbon nanotubes on 2D-semiconductor**

Yun-Hi Lee, Je-Min Yoo, Jung-Ah Lee, B. K. Ju *Good electron emitter  
Maagnetisms in CNT-S junction*

**Poster XIX.9 *Selective replacement on SiO<sub>2</sub>,  
chromophore functionalization -> photo-transistors***

**Poster XIX.10 Surface passivation of carbon nanotube field-effect transistors**

Hideki Shimauchi, Yutaka Ohno, Shigeru Kishimoto, and Takashi Mizutani

*SiO<sub>2</sub>/PMMA passivation -> reduction of hysteresis more than a month!!*

**CNT device is also seen in Poster XXI. 28, A contact/resistance issue.**

**Poster XXI.28 Electrical Resistance and Contact Properties of Carbon Nanotube Coated Surfaces**

Onnik Yaglioglu, Anastasios John Hart, Alexander H. Slocum

**Poster XXI.2 THEORETICAL AND EXPERIMENTAL STUDIES OF CARBON NANOTUBES: A REVIEW**

Katya M. Simeonova, Ganka M. Milanova

**Poster XXI.3 Sorting carbon nanotubes via dielectrophoresis**

R. Krupke, F. Henrich

**Sort metallic tube only by high-frequency field**

**Poster XXI.4 Atomic scale modelization of the nucleation of C-SWNT**

towards atomic **TB-MD and MC grand canonical->growth on (100)(111) surface**

H. Amara, C. Bichara, J.-P. Gaspard and F. Ducastelle

**Poster XXI.5 An alternate mathematical model for single-wall carbon**

nano

**New insight on nanotube structures and higher-symmetry representation**

Nicolas Collas

**Poster XXI.6 Direct structuring of single-walled carbon nanotube (SWNT)**

free standing thin films using e-beam and focused ion-beam (FIB).

S. Malik, C. A. Volkert, H. Rösner, O. Kraft , **No intermediate steps of fabrication**

**Poster XXI.7 A theoretical study of curvature effects in defective**

nanotubes

**Curvature assisted defect formation and reactivation**

Johan M. Carlsson and Matthias Scheffler

**Poster XXI.8 STRUCTURAL INVESTIGATION OF NANOTUBE CARPETS AND FIBERS AT THE MICROMETER SCALE USING SYNCHROTRON MICROFOCUS X-RAY DIFFRACTION**

V. Pichot, M **Analysis of catalytic particle from the root to top of the nanotubes**

Burghammer, C. Riekkel and P. Launois

**Poster XXI.9** Influence of monoatomic steps of nickel during the nucleation of C-SWNTs **TB-MD and Monte Carlo-grand canonical approach**  
H. Amara, C. Bichara and F. Ducastelle

**Poster XXI.10** Ion irradiation induced B/N implantation onto carbon nanotubes **Substitution of C with N/B atom: effect of later annealing: MD!**  
J. Kotakoski, A. V. Krasheninnikov, Y. Ma, A. S. Foster, K. Nordlund, and R. M. Nieminen

**Poster XXI.11** The Adsorption of Hazardous Organic Compounds onto Carbon Nanotubes Synthesized by Thermal Pyrolysis **Performance of MWNTs prepared by the thermal pyrolysis method!**  
N. J. Jeong, et al.

**Poster XXI.12** Location Control of the Growth of Carbon Nanotubes using Focused Ion Beam Selective Milling **Etched pattern on SiO<sub>2</sub> and growth**  
E. S. Sadki, S. Ooi, and K. Hirata

**Poster XXI.13** Novel actuator with single-wall carbon nanotubes as actuating material **Charge-induced forces on 10<sup>13</sup> aligned SWNTS!**  
T. Koker, U. Gengenbach, G. Bretthauer

**Poster XXI.14** Production and investigation of composition, structure and properties of fullerene-like structures' metal derivatives  
K.B.Zhogova, B. S.Kaverin, A.G.Zvenigiridskii, A. M.Ob`edkov, G.A.Domrachev, S. N.Titova, A.I.Kirillov, M.A.Lopatin, M.V.Tatsenko, Yu.V.Ignat'ev, C.N.Kortanov

**Structural analysis by Mass, EPR, NMR, X-ray, Raman...**

**Poster XXI.15 Molecular Dynamic Simulations of Single-Wall Carbon Nanotube CVD Growth** **Refined parameter for GROMOS-> T, catalysis-size dep.**  
Ali Izadi-Najafabadi, Walter R. P. Scott, and John D. Madden

**Poster XXI.16 In situ characterization of field emission from individual carbon nanotubes in the scanning electron microscopy**

Do-Hyung Kim, Chang Hyeong-Rag Lee **Alignment under applied E-> non-FN to FN emission**

**Poster XXI.17 Gas Phase Electrophoresis of Carbon Nanotubes grown in Low Pressure CVD process.** **Apply E in order to separate SWNT, MWNT, M-D.V. Smovzh, V.A. Maltsev, O. particle,  $\alpha$ -C from product.**

**Poster XXI.18 Synthesis of silicon carbide nanomaterials using multi-walled carbon nanotubes as templates** **Start from MWNT + S powder-> graphite heater 2000K!**  
V.G. Sevastyanov, A.V. Al

A.M. Ob`edkov, B.S. Kaverin, A.A.Zaitsev, K.B.Zhogova

**Poster XXI.19 NMR INVESTIGATIONS ON ALKALI INTERCALATED CARBON NANOTUBES** **Pure metallization and preferential alkali sites!**

M. Schmid, C. Goze-Bac, T. Wragberg, M. Mennig, S. Roth

**Poster XXI.20 Electrostatics of individual SWNTs investigated by EFM**

M. Paillet, P. Poncharal and A. Zahab

**Static charge distribution on INDIVIDUAL CNT on SiO<sub>2</sub>/Si**

**Poster XXI.21 Complement activation and protein adsorption by carbon nanotubes** **First-time report of activation of human complement!**

Carolina Salvador-Morales, Emmanuel Fianaut, Edin Sim, Jeremy Sloan, Malcolm L.H.Green, Robert B.Sim

**Poster XXI.22 SWNT Fluorescence Spectrum Changes Induced by Light-Assisted Oxidation** **Light-induced burning/removal of CNT with H<sub>2</sub>O<sub>2</sub>**

Minfang Zhang, Masako Yudasaka, Sumio Iijima

**Poster XXI.23 LCVD of Carbon Nanotubes, Catalytically Grown on Iron-Based Nanostructures Prepared by Laser Pyrolysis**

I. Morjan, R. Al **Laser induced CVD on catalysis/Si-sub. Checked by SEM,TEM,,, Scarisoreanu, I. Vaida, V. Ciupina, R. E. Morjan**

**Poster XXI.24 Low energy instabilities of small-radius zig-zag nanotubes**

E. Perfetto and J. Gonzalez **Coulomb-repulsion vs e-phonon-mediated attraction**

**Poster XXI.25 Photoemission of insulator-coated carbon nanotubes**

SeGi Yu, Jungna Heo, **Optimization of insulator layer for high-emission Kim (local E assisted enhancement)**

**Poster XXI.26 Local Modification and Characterization of the Electronic Structure of Carbon Nanotubes** **H-impact induced structural change**

Gilles Buchs

**Poster XXI.27 Determination of Nanotube Density by Gradient Sedimentation**

Qi Lu, Ga **Mass/Volume of bundles tends to match a geometrical simple model.**

**Poster XXI.28 Electrical Resistance and Contact Properties of Carbon**

**(CNT film)/(Au contact) has been tested-> reduction of  $\rho$  by annealing and press**

Onnik Yagilloglu, Anastasios John Hart, Alexander H. Slocum

**Poster ) Mechanisms of electromigration of inner Fe atoms is addressed**

L. de Kn **from cross-sectional structure by TEM**

**Poster XXI.30 Fractal Analysis of Carbon Nanotubes by means of Electrochemical Methods**

Ali Eftekhari, Fathollah Moztarzadeh, Parvaneh Jafarkhani

**Poster XXI.31 Structural, Electronic and vibrational properties of atomic carbon nanowires.**

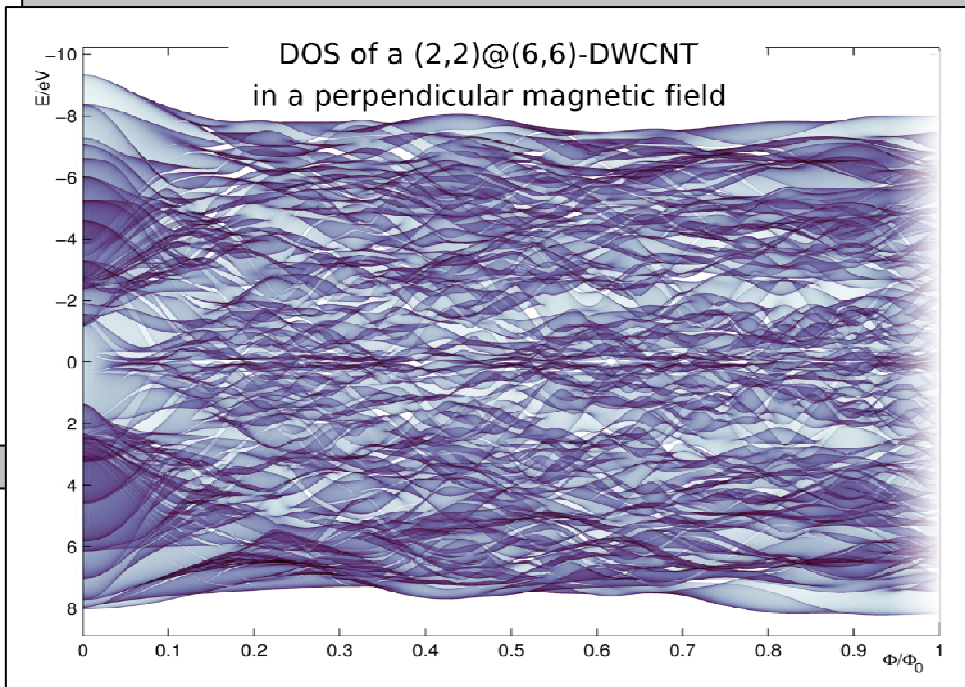
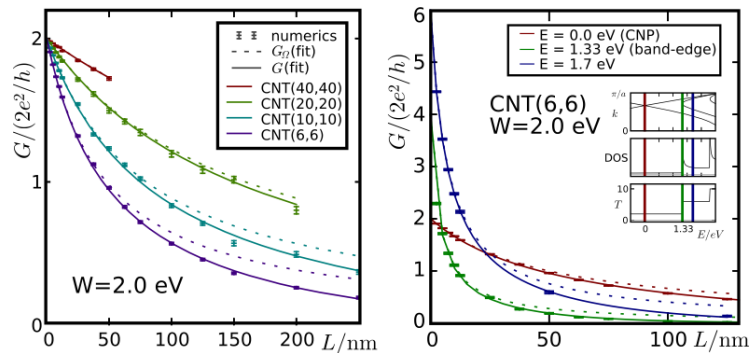
E. Cruz-Silva, M. Terrones, F. López-Uría, E. Muñoz-Sandoval<sup>1</sup>, H. Terrones, R. Saito, M. Dresselhaus, M. Endo.

## Magnetoconductance in Disordered Carbon Nanotubes

Norbert Nemeč and Gianaurelio Cuniberti

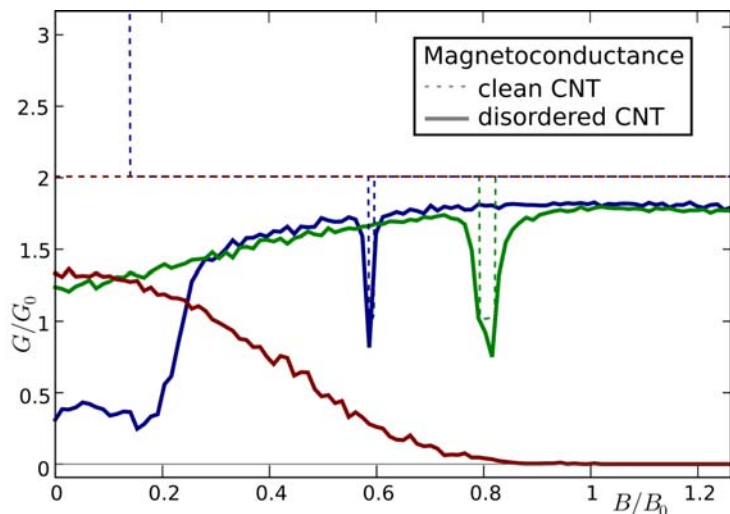
**TB& disordering**

Length dependence of conductance



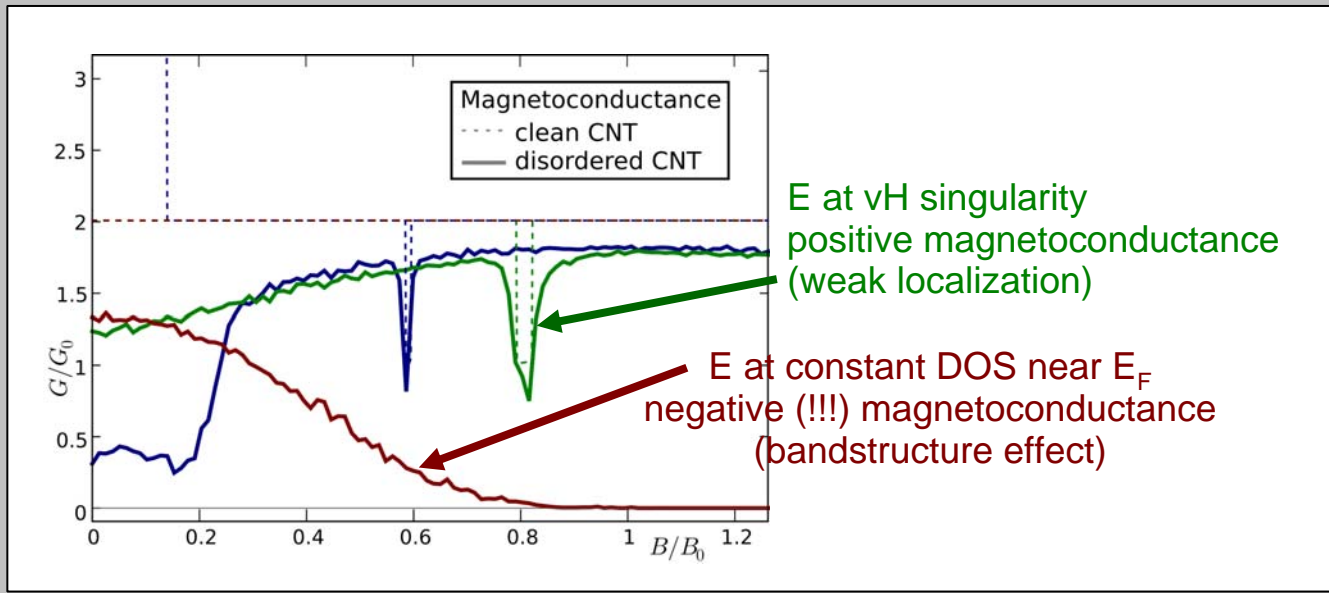
positive magnetoconductance  
(weak localization)

negative (!!!) magnetoconductance  
(bandstructure effect)



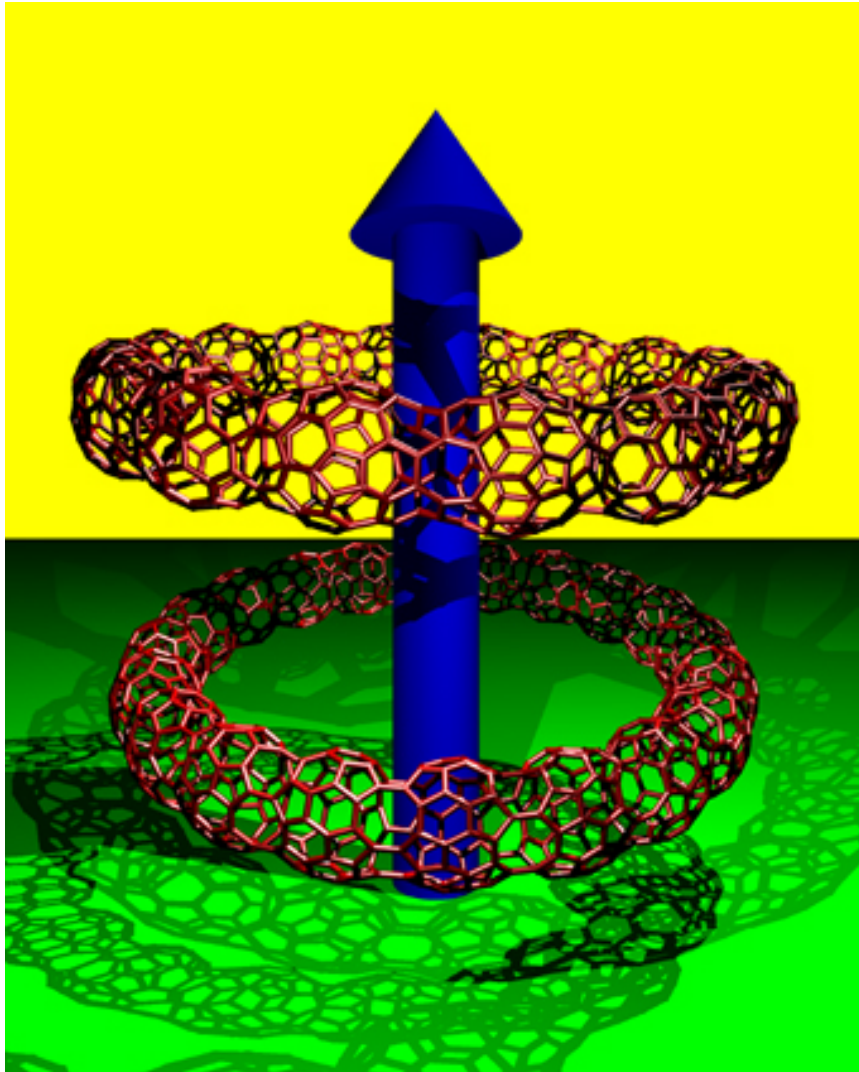


# XX.2



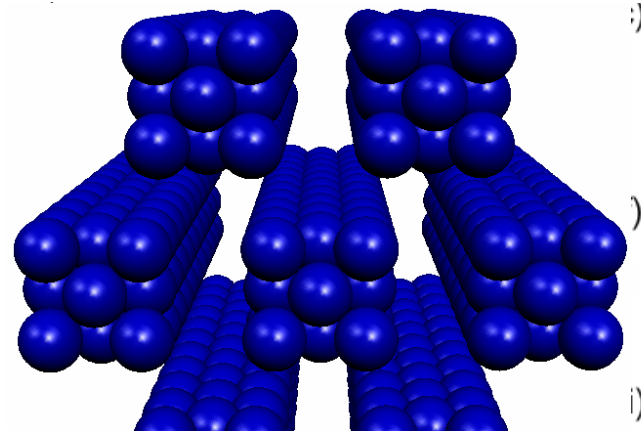
# Magnetism in Carbon and Metal Nanowires

## Ring Currents in Carbon Toroids

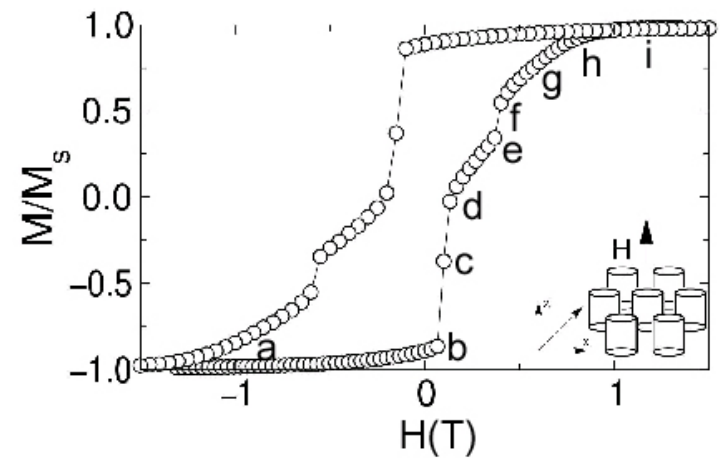


Poster XX.6

## Magnetization Studies of Fe NWs



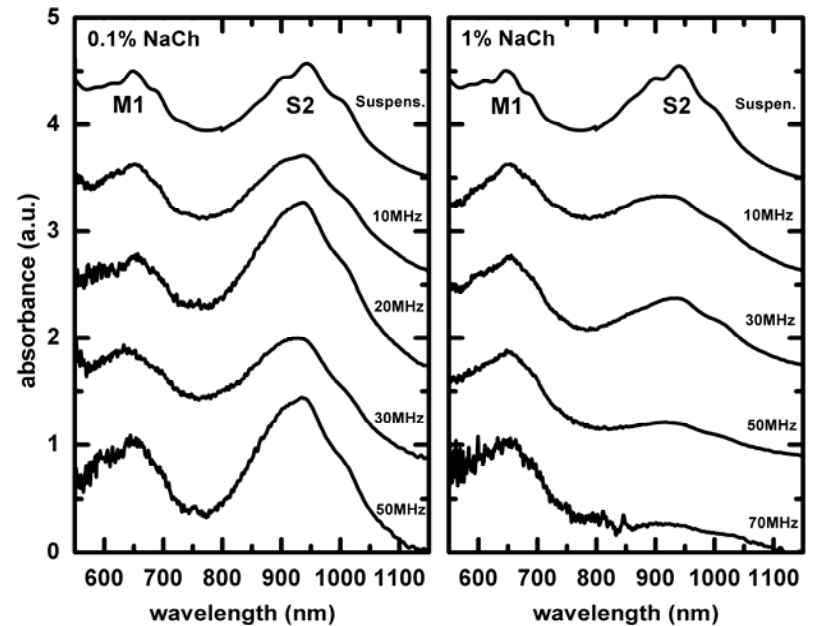
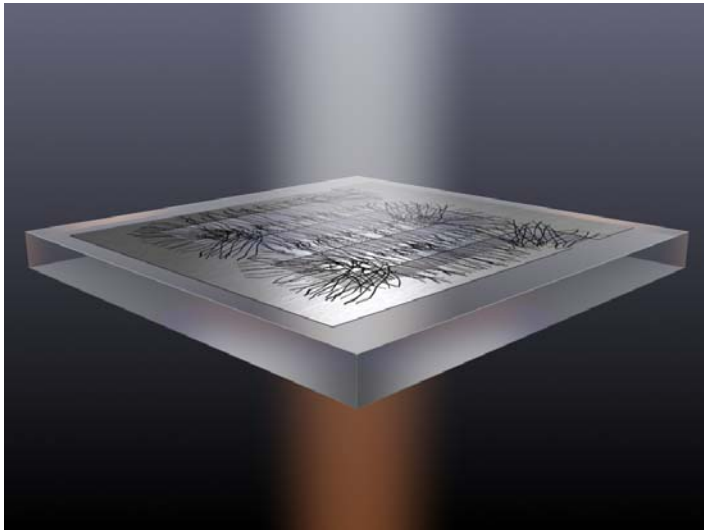
**Helical alignment of spin inside NT?!  
Checked by Exp. And Theory**



Poster XX.7

## Sorting carbon nanotubes via dielectrophoresis

*R. Krupke, F. Henrich*



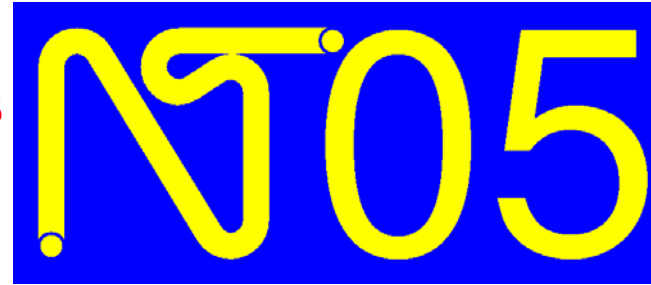
Optical absorption spectra confirm our previous Raman data:  
**Metallic tubes are separated from semiconducting tubes by  
 high-frequency, high-field dielectrophoresis – for all diameters !**

**NT05: Sixth International Conference on the  
Science and Application of Nanotubes**

***Göteborg, Sweden***

***June 26 - July 1, 2005***

**<http://nanotube.msu.edu/nt05/>**



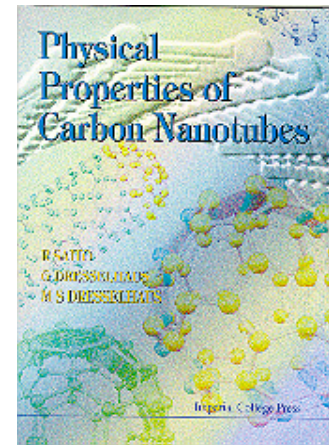
**CR Mildred Dresselhaus Friday, July 1**

**Concluding Remarks**

# Outline

M. Terrones & M.S. Dresselhaus

- **Conference Overview**
- **What we learned at NT05**
- **Achievements and Trends**
- **Challenges & Future Work**



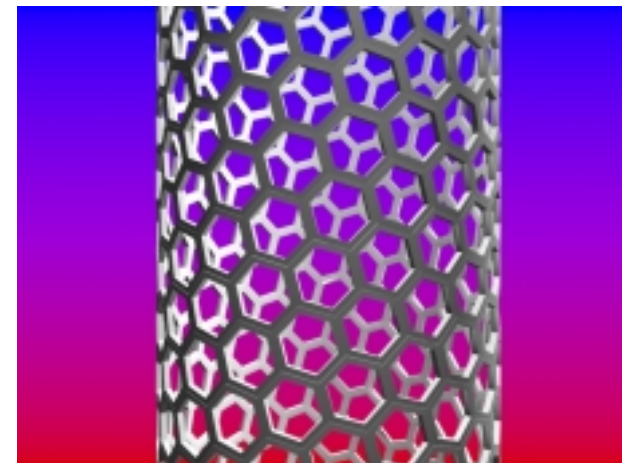
*“Physical Properties of Carbon Nanotubes”*,

by R. Saito, G. Dresselhaus and M.S. Dresselhaus,  
Imperial College Press (1998) ISBN 1-86094-093-5

# Conference Overview

Time	Sun 26	Mon 27	Tues 28	Wed 29	Thurs 30	Fri 1
08:30-09:00		Registration	Registration			
09:00-09:45			Maurizio Prato	Morinobu Endo	David Tomanek	Paul McEuen
09:45-10:15		Welcoming address (09:30-10)	Alan Windle	Susumu Katagiri	Jean-Louis Sauvajol	Nadine Kam
10:15-10:45		Sumio Iijima (10-10:45)	Jerry Tersoff	Jean Dijon	Junichiro Kono	Cheol Jin Lee
10:45-11:15		Steven Louie	Coffee	Coffee	Coffee	Coffee
11:15-11:45		Coffee	Young Hee Lee	Jong-Min Kim	Tony Heinz	Brian LeRoy
11:45-12:05		Humberto Terrones (11.45-12.15)	Yoshinori Sato	Atsuko Nagataki	Arkady Krashennnikov	SangWook Lee
12:05-12:25		Lars Samuelson (12.15-12.45)	Lunch	Anna Swan	Lunch	Lunch
12:25-14:00		Lunch (12.45-14.20)		Lunch		
14:00-14:20			Pavel Nikolaev	Boat trip and conference dinner	Gotthard Seifert	Pertti Hakonen
14:20-14:40		Feng Ding	Vincent Jourdain		Bo Gao	Andrew Wall
14:40-16:00		Masahiko Ishida (14.40-15)	Poster session A		Poster session B	Poster session B
16:00-18:00		Registration	Chair A.2 14:40-14:45 Chair A.3 16:30-16:35 Chair A.4 18:30-18:35		Chair B.1 14:40-14:45 Chair B.2 16:30-16:35 Chair B.3 18:30-18:35	Chair B.4 14:40-14:45 Chair B.5 17:00-17:05
18:00-19:00		Welcome party				Snacks 19:00
19:00-21:00	Göteborg city reception				Concluding remarks 20:00	

N05



# **NT05** Conference Overview

→ *CVD Synthesis of Carbon Nanotubes* (81)

*Non-CVD Synthesis of Nanotubes* (17)

Formation and Characterization of Unusual Nanostructures (14)

*Raman Characterization of Nanotubes* (12)

*Other Characterization of Nanotubes* (18)

*Nanotube Dispersion and Purification* (9)

→ *Chemical Modification of Nanotubes* (29)

*Non-Carbon Nanotubes* (12)

→ *Nanotube-Based Composites* (26)

Morphology and Application of Modified Nanotubes (13)

*Photo-Induced Reactions in Nanotubes* (1)

Thermal and Mechanical Properties of Nanotubes (16)

*Atomic Structure of Carbon Nanotubes* (10)

→ *Transport in Nanotubes* (37)

*Field Electron Emission* (14)

→ *Optical Properties and Optoelectronics* (24)

*Transport in Complex Nanostructures* (4)

Electron-Phonon Coupling in Complex Nanostructures (2)

*Nanotube-Based Transistors* (10)

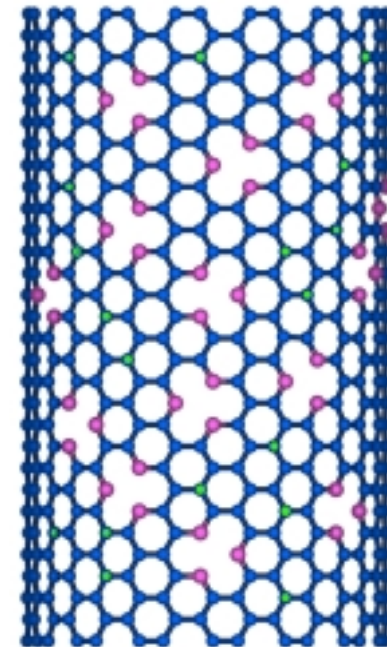
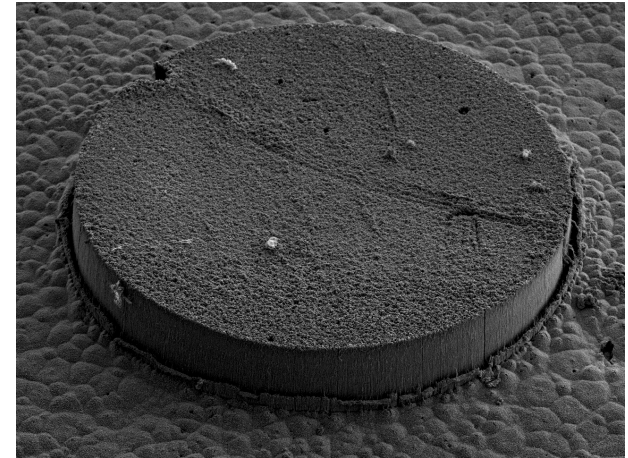
*Magneto-Transport and Magnetism* (5)

General Studies of Carbon Nanostructures (31)

**(402 contributed abstracts received in total)**

# CVD and Non-CVD Techniques

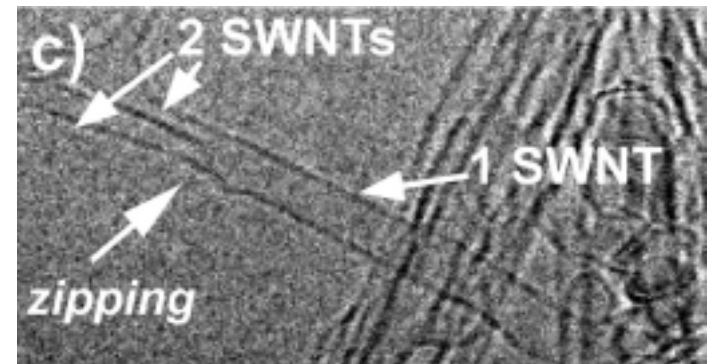
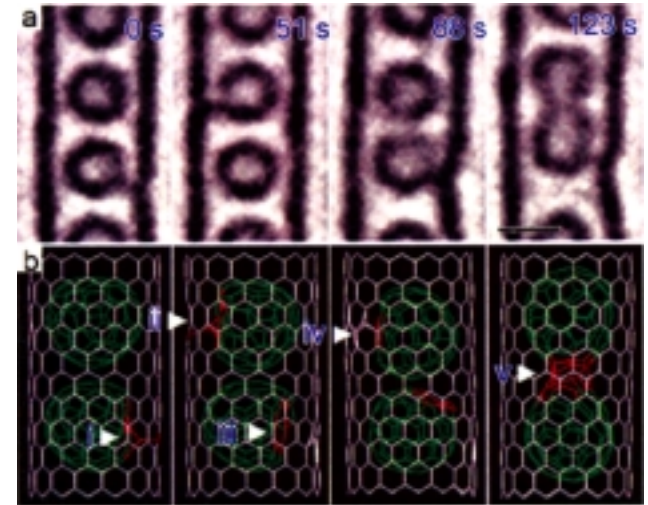
- CVD method is developing fast
  - **Bulk Production** and Scalable Process (companies developing).
  - **Alcohol** based CVD is powerful
  - **Continuous spinning** of Nanotube Fibers
  - **More active & controlled effort on DWNTs**
  - Starting Effort on **triple-walled NTs**
  - **Alignment** of nanotube arrays MWNTs (multi-layers)
  - **Supergrowth** Mechanism with H<sub>2</sub>O (SWNTs)
  - **Doped Nanotubes**
- Plasma-enhanced CVD → Now making SWNTs
- No chirality Control yet!! But beginning!!
- More emphasis on **Small Diameter Tubes**
- Non-CVD (Arc, Magnetron Sputtering, Chemical, Laser, Ball-Milling)





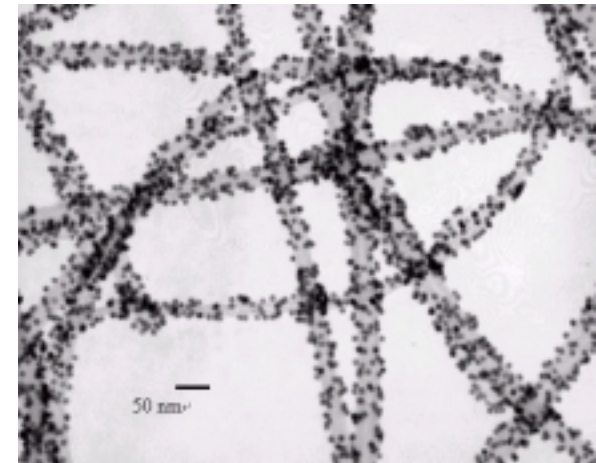
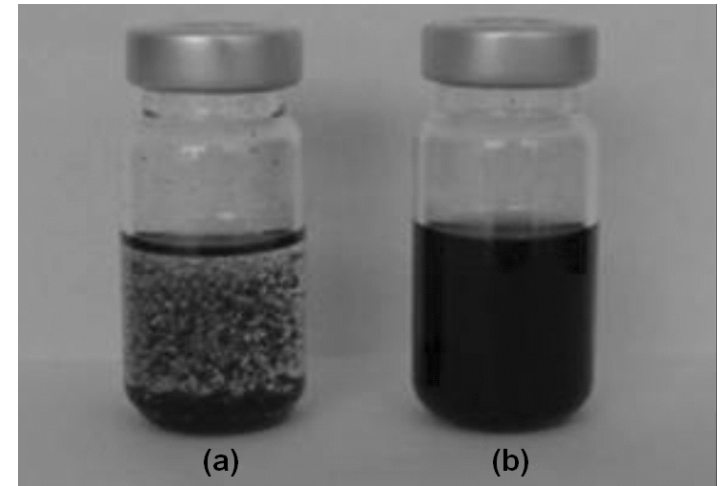
# Characterization

- HRTEM is improving (useful and powerful)
  - Defects (individual atoms, vacancies)
  - Chirality (n,m) by imaging and ED
  - In-situ experiments (growth, kinetics)
- Catalyst-NT Membranes under HRTEM → growth process
- MD simulations of NT growth
- Raman Spectroscopy
- STM and STS
- Photo-luminescence
- Magnetic Force Microscopy  
Developing Fast



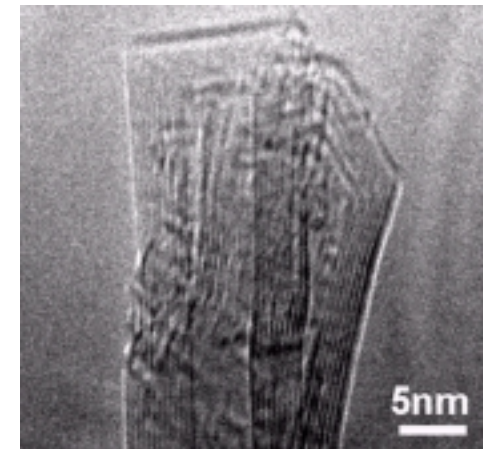
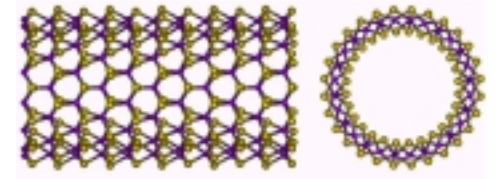
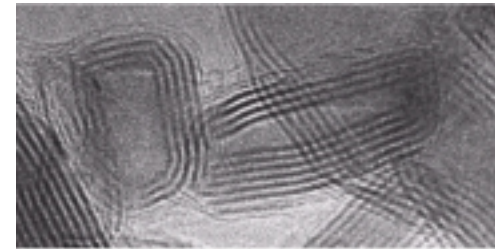
# Chemistry of Nanotubes

- Graphite and large diameter NTs are inert
- Introducing activity → Defects
- How to quantify and identify defects (Novel Electrochemical Methods)
- Functionalization & Dispersion Methods
- Separating, Cutting and positioning NTs.
- Doped Nanotubes
- Sensors and Biosensors
- Patterned growth of SWNTs on sapphire step surfaces
- DNA-wrapped tubes, Fluorination
- Removing amorphous carbon, and metal particles, adsorbates



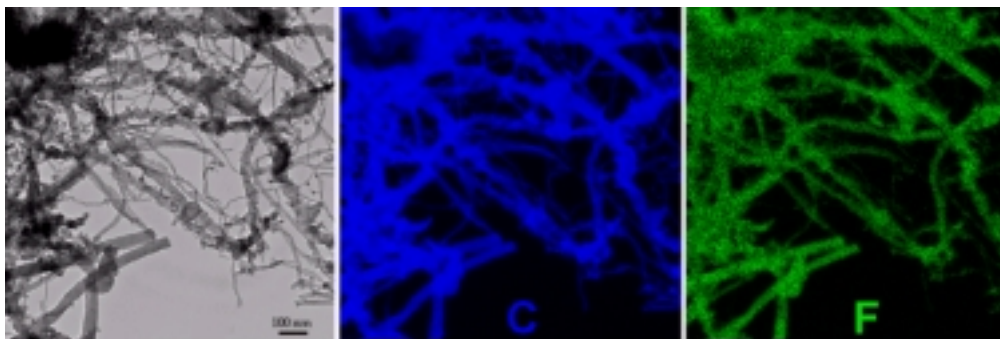
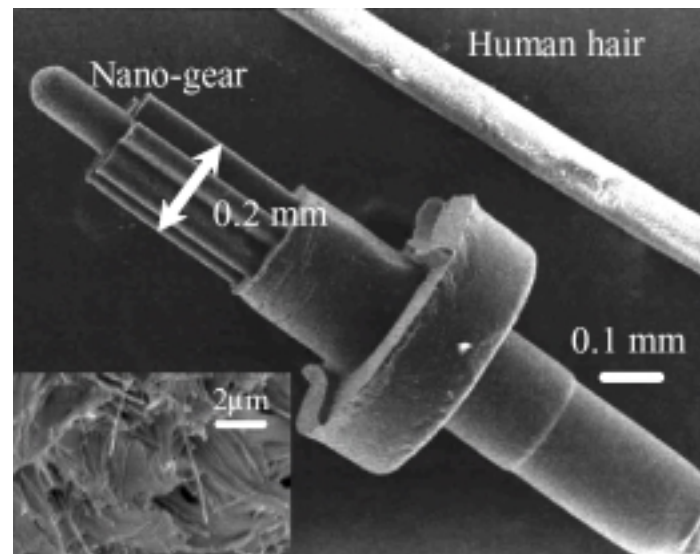
# Non-Carbon Nanotubes, Nanowires & Related Materials

- BN, BCN Nanotubes
- Defects in BN tubes
- Nanotubes (layered Materials)
  - TiO<sub>2</sub>, MoS<sub>2</sub>, WS<sub>2</sub>, CdS, etc.
- Need Calculations
- More Synthesis methods of layered nanotubes.
- More Property Measurements
- Nanowires of CdSe, ZnSe, ZnO, Si, BiSb, etc.
- *Future Trends: More Nano-Bio & Nano-graphite*



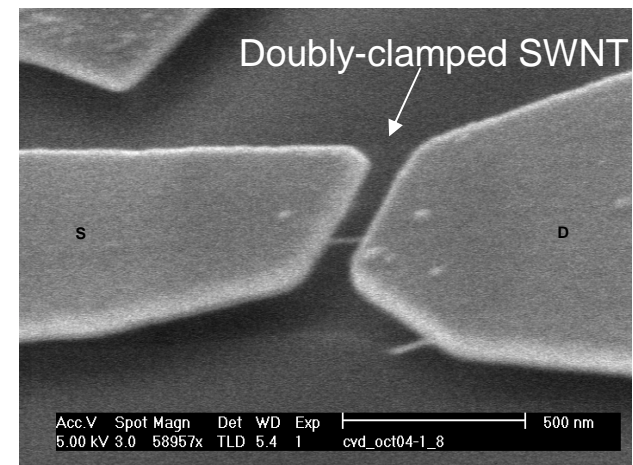
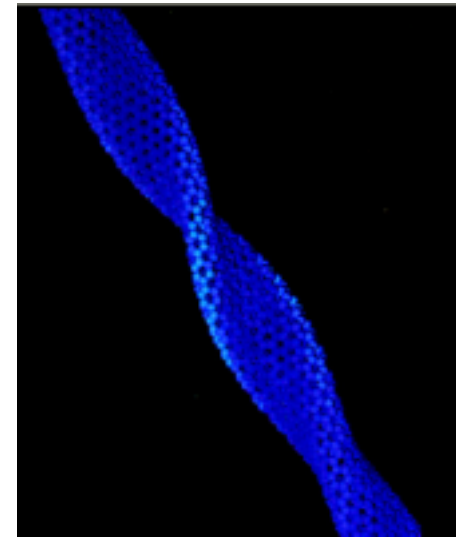
# Composites and Modified Tubes

- Polymer Composites (we need standards)
- Conducting Polymers (transparent films)
- Electro-spinning of fibers
- In-situ polymerization from NT wall
- Novel Composites:  
Liquid Crystal,  
Ceramic-NT  
Metal-NT



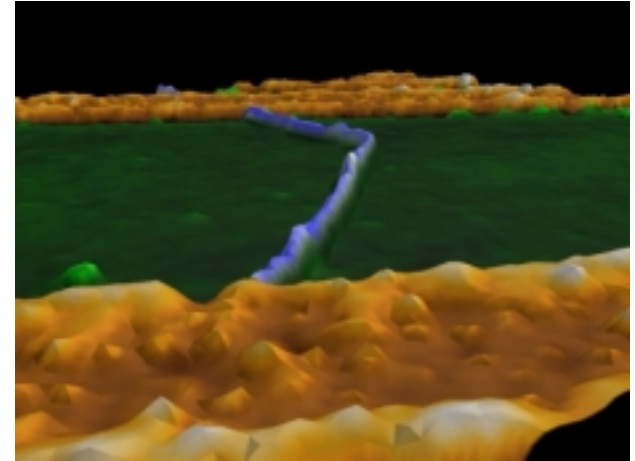
# Mechanical and Structural Properties

- Confinement effects of any filler within tubes (liquid, gas, solid)
- Current induced bends, repairing structural defects
- Generation & Disappearance of Stone-Wales type defects.
- Controlled point defects and their mobility
- Starting to do more NEMS with NTs
- Faceting MWNTs with Temperature
- Kohn Anomalies (Theory & Exp.)



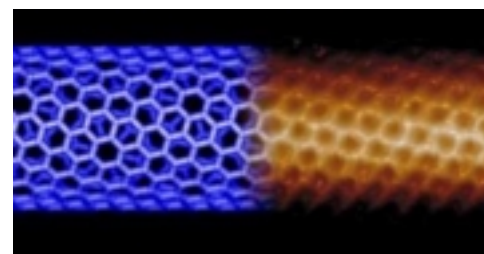
# Transport in Nanotubes

- Devices from using long tubes provide better values for carrier scattering and mobility
- Firm evidence for phonon scattering effects in transport, and separation of acoustic and optical phonon contributions
- Measurements on suspended NTs (eliminate some extrinsic behaviors)
- Detailed understanding of SET and Kondo effects
- Combining Transport with Raman, etc
- Studies of Noise starting...
- *Still to come: Detailed understanding of Disorder & Defects in Transport*
- *Transport of DWNTs*



# Photophysics

- Two-photon absorption experiments (Columbia & Berlin groups) demonstrated the need for excitons.
- Details of the exciton picture to describe the photophysics of SWNTs are emerging rapidly, including optically active and dark states.
- Correspondence principle between the usual Kataura plot and exciton model has been introduced.
- Femtosecond optics reveals lifetime of selected excited states, clarifying exciton picture.
- Coherent phonon generation in nanotubes has been demonstrated
- Rayleigh scattering for (n,m) determination



# Applications

- **Polymer Composites**  
**High Thermal Conducting Plastics**  
**Conducting Paints for automobiles**  
**Micro-gears**
- **Li-ion batteries & Lead acid batteries**
- **Field Emission Devices & Displays**
- **Nanotube-based Transistors**
- **Biological Applications**  
**Micro-catheters, protein immobilizers, Drug Delivery, Cancer treatment**
- **We need more COMMERCIAL APPLICATIONS**

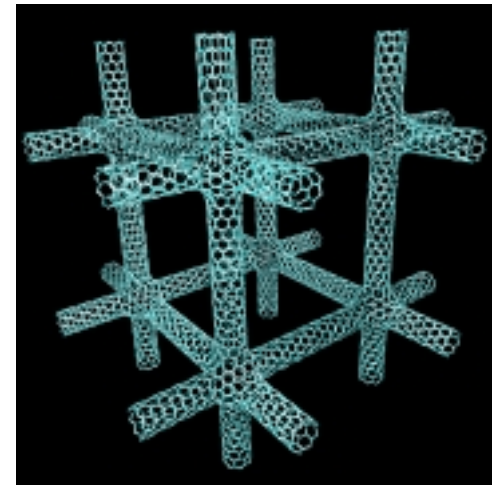




# Overall Challenges

- **Standards**

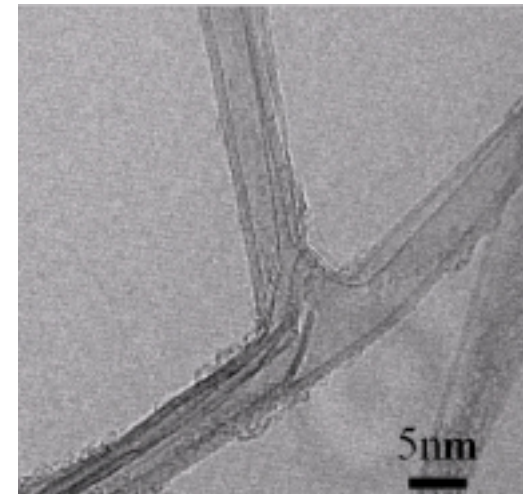
- On materials Characterization
- How good are SWNTs, DWNTs, MWNTs?
  - Mean Diameter and distribution
  - Mean length and distribution
  - amorphous carbon content
  - Other materials content
  - Determine Metal/Semiconductor ratio
  - Determine (n.m) distribution
  - Identify Defect contents
  - Determine Functional groups
  - Estimate Doping
  - Bundles? Size of bundles?
- How to BEST determine these parameters?
  - Combination of HRTEM, Raman, PL, TGA, SPM, etc.
- Establish parameters for best qualities, set minimum standards for applications, what accuracy is needed?



# Overall Challenges

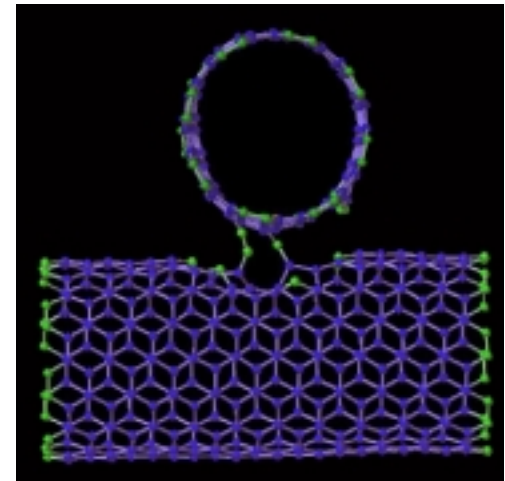
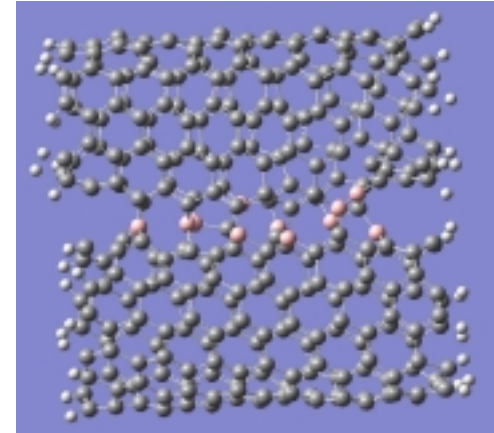
- **Health Effects**

- Present status and knowledge
- Best handling practices
- Effects on skin, lungs, etc.
- Carcinogenic effects?
- What studies need to be done?
- New special issue on Toxicity (Carbon Journal)



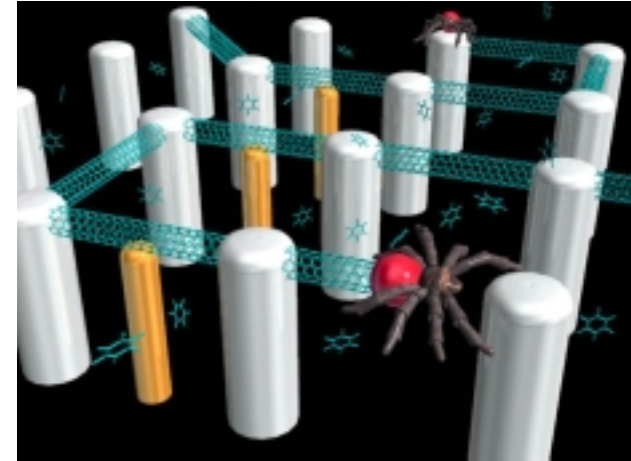
# Theoretical Challenges

- Need accurate Calculations for NT growth (large scale in space and time)
- Theory on Chemistry of NTs
  - Effect of Functionalization on electronic & transport properties
  - Doping Effects
- Effect of Specific Defects on electronic properties & structural stability
- Electronic and Geometric Structure of DWNTs (treating incommensurability)
- Exciton Calculations for Photophysical Properties
- Predicting New Materials for Functionality & New Physics



# We need to work on...

- **Real control of nanotube growth (catalyst dimensions and chirality selectivity)**
- **Improve Characterization Techniques**
- **In-situ experiments and at the individual NT level**
- **Easy NT manipulation**
- **Thermal Transport on individual NTs**
- **More experiments that are definitive of exciton phenomena including identification of dark states**
- **Applications**



# Future NTxx Conferences

- NT06 in Japan
- NT07 in Brazil
- NT08 ??? – please post advert on Forum