II. International Workshop on the Science and Application of Nanotubes

July 22-25, 2001

Inselhotel Hermannswerder

Potsdam, Germany

When Angels breathe

By Peter Butzloff, University of North Texas

Who's heard of the shifty pretty lady
in charge of wicks small and shady?
This lass with the clay and poles,
she peers at her land of holes.

I write to this pretty shifty lady
amongst her sticks nanosuedey
who reads of my word in scrolls
and feels of the finest coals.

My outline is really straight and simple
of nanotubes bound to dimple
the commonest ground to be
at commonly bent degree.

Sticks mix with the swollen clay so braidy
as bonelike wicks grown quite jady.
Sincere as an inverse cube
in shear is a nanotube.

She stares at the glade where ended daisy.
Can blaze of bush burnt upraise thee?
This lady of shifty knolls
calls angels to breathing coals.

Workshop Organization:

Tobias Hertel (Fritz-Haber-Institut der MPG)
Angel Rubio (DIPC San Sebastian)
David Tománek (Michigan State University)

International Board of Advisors:

Phaedon Avouris (IBM Yorktown Heights)
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Major Sponsoring Organizations:

Office of Naval Research International Field Office, Office of Naval Research Headquaters, USAF European Office of Aerospace Research and Development

Deutsche Forschungsgemeinschaft (DFG)

Max-Planck-Gesellschaft (MPG)

Further Support was Provided by:

Asian Technology Information Program (ATIP)

State of Brandenburg; Ministry of Science, Research and Culture

Nantubulites Project (NEC Corporation)

PHANTOMS, IST Nanotechnology Network

NanoLab, Boston

Institute of Physics Publishing

Springer Verlag, Heidelberg

Special Thanks to:

Kirstin Hertel-Dietrich
Lisa Maier
Mirjam Meyer
Gunnar Moos
Rosa Stottko
Hendrik Ulbricht
Renju Zacharia

Welcome to Nanotube 2001

The success of the first International Nanotube Workshop at the Michigan State University in 1999, encouraged us to set out on this journey and organize the second meeting of its kind: Nanotube 2001. It is our hope that this will be the beginning of an inspiring and successful series of workshops within a unique field that has caught the interest and imagination of many of us over the past 10 years.

This workshop is intended to provide a platform to exchange the latest results of your scientific work, your ideas and your visions of this rapidly developing field within an informal atmosphere. Poster sessions and invited presentations will play an equally important role for the meeting and will facilitate a lively discussion on a variety of topics associated with the latest developments in nanotube science.

With all the best for a stimulating and exciting meeting.

(Tobias Hertel)

(Angel Rubio)

(David Tománek)

Arrival & Departure

Saturday, July 21	Sunday-Wednesday, 22-25 July	Thursday, July 26
Arrival, Welcome reception (18:00-21:00)	Scientific Program	Breakfast (6:30-10:00), Departure

Program Timetable

	Sunday, July 22	Monday, July 23	Tuesday, July 24	W-day, July 25
6.30 – 8.30	BREAKFAST	BREAKFAST	BREAKFAST	BREAKFAST
8.30 – 10.00	Welcome Address & Session Su1	Session Mo1	Session Tu1	Session We1
10.00 – 10.30	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	COFFEE BREAK
10.30 – 12.00	Session Su2	Session Mo2	Session Tu2	Session We2
12.00 – 13.30	LUNCH	LUNCH	LUNCH	LUNCH
13.30 – 15.00	Session Su3	Session Mo3	Session Tu3 COFFEE BREAK	Session We3
15.00 – 15.30	COFFEE BREAK	COFFEE BREAK	Poster-PLUS contributed talks and posters PoS Tu	COFFEE BREAK
15.30 – 18.30	Poster-PLUS contributed talks and posters PoS Su	Poster-PLUS contributed talks and posters PoS Mo		Poster-PLUS contributed talks and posters PoS We
18.30 – 20.00	DINNER	DINNER	Boat/Bus trip & Banquet (ends 22-24:00)	DINNER
20.00 – 21.00	Poster Session PoS Su (continued)	After Dinner Presentation		Poster Session PoS We (continued)
21.00 – 22.00				

Program

Sunday 22 July 2001

6.30 - 8.30	BREAKFAST
Session: Su1	Chair: **Mildred S. Dresselhaus**
8.30 - 8.40	Welcome address
8.40 - 9.25	**Sumio Iijima** (Meijo University and NEC) *Single-Wall Graphite Sheets as Molecule Adsorption*
9.25 - 10.10	**Annick Loiseau** (LEM, Châtillon) *Root Growth Mechanism for Single Wall Nanotubes*
10.10 - 10.30	COFFEE BREAK
Session: Su2	Chair: **Richard Martel**
10.30 - 11.15	**Jim Hone** (CalTech) *Thermal Properties and Quantized Phonon Spectrum of Single-Walled Carbon Nanotubes*
11.15 - 12.00	**Laszló Fórró** (EPF Lausanne) *Disorder and Pressure Effect on the Physical Properties of Carbon Nanotubes*
12.00 - 13.30	LUNCH
Session: Su3	Chair: **Steven G. Louie**
13.30 - 14.15	**Marc Bockrath** (Harvard) *Transport in Carbon Nanotubes*
14.15 - 15.00	**Reinhold Egger** (Universität Düsseldorf) *Spin Transport and Coulomb Blockade in Nanotubes*
15.00 - 15.30	COFFEE BREAK
Poster-PLUS Session: PoS Su	Chair: **David Tománek**
15.30 - 18.30	Contributed talks and posters
18.30 - 20.00	DINNER

Monday 23 July 2001

6.30 - 8.30	BREAKFAST
Session: Mo1	Chair: **Peter C. Eklund**
8.30 - 9.15	**David Luzzi** (UPenn) *Carbon Nanotube-Based Hybrid Materials*
9.15 - 10.00	**Robert Schlögl** (Fritz-Haber-Institut) *Carbon Nanomaterials in Heterogeneous Cataylsis*
10.00 - 10.30	COFFEE BREAK
Session: Mo2	Chair: **Laszló Fórró**
10.30 - 11.15	**Philip G. Collins** (IBM, T.J. Watson Research Center) *Controlling the Electronic Properties of Carbon Nanotube Bundles*
11.15 - 12.00	**Walt A. de Heer** (Georgia Tech) *When are Carbon Nanotubes Ballistic Conductors*
12.00 - 13.30	LUNCH
Session: Mo3	Chair: **Susumu Saito**
13.30 - 14.15	**Cees Dekker** (Delft University of Technology) *Recent Transport and STM Results on Carbon Nanotubes*
14.15 - 15.00	**Steven G. Louie** (Berkeley) *Theoretical Study of the Quantum Conductance of Nanotube Structures: Defects, Junctions, and Peapods*
15.00 - 15.30	COFFEE BREAK
Poster-PLUS Session: PoS Mo	Chair: **Marc Bockrath**
15.30 - 18.30	Contributed talks and posters
18.30 - 20.00	DINNER
After Dinner Presentation	Chair: **Tobias Hertel**
20.00 - 21.00	**Mildred S. Dresselhaus** (MIT) *Perspectives on the Role of Carbon Nanotube Research in the Worldwide Nanotechnolgy Initiative*

Tuesday 24 July 2001

6.30 - 8.30	BREAKFAST
Session: Tu1	Chair: **David Luzzi**
8.30 - 9.15	**Mauricio Terrones** (University of Sussex & UNAM) *Novel Layered Nanomaterials: Controlled Synthesis, Electronic Properties and Applications*
9.15 - 10.00	**Hiromichi Kataura** (Tokyo Metropolitan University) *Optical Properties of Fullerene- and Non-Fullerene-Peapods*
10.00 - 10.30	COFFEE BREAK
Session: Tu2	Chair: **Jerry Bernholc**
10.30 - 11.15	**Mark Golden** (IFW Dresden) *The Optical Properties and Electronic Structure of SWCNT: Empty, Stuffed or Surrounded by Dopants*
11.15 - 12.00	**Peter C. Eklund** (Penn State University) *Molecule/SWNT Interactions: Effects on Electronic and Phonon Properties*
12.00 - 13.30	LUNCH
Session: Tu3	Chair: **Louis Schlapbach**
13.30 - 14.15	**Robert C. Haddon** (Riverside) *Chemistry of Single-Walled Carbon Nanotubes*
14.15 - 14.45	COFFEE BREAK
Poster-PLUS Session: PoS Tu	Chair: **Jim Hone**
14.45 - 17.30	Contributed talks and posters
18.00 - 24.00	BOAT/BUS-TRIP & BANQUET

Wednesday 25 July 2001

6.30 - 8.30	BREAKFAST
Session: We1	Chair: **Philippe Lambin**
8.30 - 9.15	**Wongbong Choi** (Samsung) *Carbon Nanotube and its Application to Nanoelectronics*
9.15 - 10.00	**Louis Schlapbach** (Universite Fribourg & EMPA) *Carbon Nanostructures: Growth, Electron Emission, Interactions With Hydrogen*
10.00 - 10.30	COFFEE BREAK
Session: We2	Chair: **Annick Loiseau**
10.30 - 11.15	**Reshef Tenne** (Weizmann Institute) *Inorganic Nanotubes and Inorganic Fullerene-Like Materials of Metal Dichalcogenides*
11.15 - 12.00	**Jie Liu** (Duke University) *CVD Synthesis of Single-Walled Carbon Nanotubes on Aerogel Supported Catalyst*
12.00 - 13.30	LUNCH
Session: We3	Chair: **Philip G. Collins**
13.30 - 14.15	**Jerry Bernholc** (North Carolina State University) *Theoretical Studies of Quantum Transport, Pyro- and Piezo-Electric Effects and Lithium Intercalation*
14.15 - 15.00	**Hongjie Dai** (Stanford) *Carbon Nanotube Molecular Wires: Recent Progress in Synthesis, Characterization and Devices*
15.00 - 15.30	COFFEE BREAK
Poster-PLUS Session: PoS We	Chair: **Mark Golden**
15.30 - 18.30	Contributed talks and posters
18.30 - 20.00	DINNER

Presentations in chronological order

Sunday, July 22, 2001: Invited talks

Su1 A **Single-Wall Graphite Sheets as Molecule Adsorption**
Sumio Iijima

Su1 B **Root Growth Mechanism for Single-Wall Nanotubes**
A. Loiseau, J. Gavillet, C. Journet, F. Willaime, F. Ducastelle and J-C. Charlier

Su2 A **Thermal Properties and Quantized Phonon Spectrum of Single-Walled Carbon Nanotubes**
James Hone

Su2 B **Disorder and Pressure Effect on the Physical Properties of Carbon Nanotubes**
Laszló Fórró

Su3 A **Transport in Carbon Nanotubes**
M. Bockrath, W. Liang, D. Bozovoc, J. Hafner, C. M. Lieber, M. Tinkham, H. Park

Su3 B **Spin Transport and Coulomb Blockade in Nanotubes**
R. Egger, A.O. Gogolin

Sunday, July 22, 2001: Poster Presentations

PoS Su1 **Qualitative and Quantitative Assessment of the SWNT Produced by the Controlled Catalytic Production Before and After Purification**
F. Pompeo, L. Balzano, H. Barraza, J. E. Herrera, E. O'Rear, S. Dahl, W.E. Alvarez, **D.E. Resasco**

PoS Su2 **Room Temperature Growth of Single Wall Coiled Carbon Nanotubes and Y-Branches**
L. P. Biró, R. Ehlich, Z. Osváth, A. Koós, Z. E. Horváth and J. B.Nagy

PoS Su3 **Defects in the Catalytic Multiwall Carbon Nanotubes**
L.G. Bulusheva, A.V. Okotrub, I.P. Asanov, A. Fonseca and J. B. Nagy

PoS Su4 **Investigation of the Growth Mechanism of Vertically Aligned Carbon Nanotubes Using High Resolution Electron Microscopy**
C. Ducati , M. Chhowalla, K.B.K. Teo, I. Alexandrou, N.L. Rupesinghe, G.A.J. Amaratunga, J. Robertson, W.I. Milne, A. Papworth, C.J. Kiely

PoS Su5 **Isotope Effects of CH_4 in Synthesis of Single-Walled and Multi-walled Carbon Nanotube by Thermal Chemical Vapor Deposition**
Fumiyuki Hoshi, Takefumi Ishikura, Kei Kikuchi, Akiko Goto, Satoshi Ohshima, Motoo Yumura, Yoshinori Koga, Shuzou Fujiwara

PoS Su6 **Optical Absorption Study of Rate-limiting Processes in the Laser Evaporation Synthesis of Single-Wall Carbon Nanotubes**
O. Jost, A.A. Gorbunov, W. Pompe, X. Liu, M.S. Golden, and J. Fink

PoS Su7 **Formation of Single- and Double-Walled Carbon Nanotubes by a CVD Method**
Ch. Laurent, A. Peigney, P. Coquay, S. Rul , E. Flahaut, E. De Grave, R. E. Vandenberghe, W. S. Bacsa, A. Rousset

PoS Su8 **Growth Mechanism of Bamboo-Shaped Carbon Nanotubes Using Thermal Chemical Vapor Deposition**
C. J. Lee, T. J. Lee, S. C. Lyu , and J. E. Yoo

PoS Su9 **Multiwall Carbon Nanotubes Grown on Metallic Substrates**
F. Kreupl, A. Graham, E. Unger, M. Liebau, W. Hönlein

PoS Su10 **Single Carbon Nanotube Raman Spectroscopy**
M.S. Dresselhaus, Ado Jorio, G. Dresselhaus, and R. Saito

PoS Su11 **Comparison of Diameter Distribution of SWCNT Bundles as Analyzed by Scanning Probe Microscopy and by Raman Measurements**
M. Mannsberger, H.Kuzmany, W.Planck, T.Pichler, A.Grüneis

PoS Su12 **Accurate Density Functional Calculations of Phonons in Carbon Nanotubes**
Orest Dubay, Georg Kresse, Hans Kuzmany

PoS Su13 **High Volume Production of Vapor Grown Carbon Nanofibers**
Xinhe Tang , Erich Leister, Ernst Hammel, Christian Nagl and Klaus Mauthner

PoS Su14 **Length Measurements and Dispersion of Isolated Single-Wall Carbon**
Pavel Nikolaev, Sivaram Arepalli, William Holmes, and Bradley Files

PoS Su15 **Identification and Properties of 4Å Smallest Carbon Nanotubes**
Lu-Chang Qin, Xinluo Zhao, Kaori Hirahara, Yoshiyuki Miyamoto, Yoshinori Ando, Sumio Iijima

PoS Su16 **Highly Selective Catalyst for Synthesis of SWNT by CO Disproportionation**
J. E. Herrera, L. Balzano, W. E. Alvarez, D. E. Resasco

PoS Su17 **Cost-Effective Controlled Production of Single-Walled Nanotubes**
W. E. Alvarez, L. Balzano, J. E. Herrera, D. E. Resasco

PoS Su18 **Gas Phase Synthesis of SWNT in an Atmospheric Pressure Plasma Jet**
Olivier Smiljanic, Barry L. Stansfield, Jean-Pol Dodelet, Alessandra Serventi

PoS Su19 **Nano-EELS Diagnoses of Hybrid Nanotubes, Nanocoils, and Nanocables**
K. Suenaga

PoS Su20 **Electron Beam Identification and Machining of Novel Hybrid Nanotubular Structures**
Trasobares S. Stephan O. C. Colliex, G. Hug, W.K.Hsu, H.W.Kroto, D.R.M. Walton

PoS Su21 **Polymer Forms of Single Wall Nanotubes**
Leonid Chernozatonskii , Madhu Menon

PoS Su22 **Excitonic-Insulating States in Carbon Nanotubes**
Freek Langeveld and Gerrit E. W. Bauer

PoS Su23 **Interwall Interaction and Charge Redistribution in Double-Wall Carbon Nanotubes**
Yoshiyuki Miyamoto, Susumu Saito, and David Tománek

PoS Su24 **A Density Functional Theory Study of Single Wall Nanotubes**
Ruth Pachter, Zhiqiang Wang, W. Wade Adams

PoS Su25 **Quantum Interferences in Carbon Nanotubes**
F. Triozon, A. Rubio and **S. Roche**

PoS Su26 **Boron Nanotubes: A Theoretical Study**
Susumu Saito and Koichiro Umemoto

PoS Su27 **On the Stability and Formation of Nanotubes**
G. Seifert

PoS Su28 **Linear Electrodynamics of Carbon Nanotubes**
S.A. Maksimenko, **G.Ya. Slepyan**, A. Lakhtakia, and O.M. Yevtushenko

PoS Su29 **Broken Symmetry, Boundary Conditions, and Band Gap Oscillations in Finite Single-Wall Carbon Nanotubes**
C.S. Jayanthi, L. Liu, and **S. Y. Wu**

PoS Su30 **Formation Mechanism and Packing of Nanotube Peapods**
Savas Berber, Mina Yoon, and **David Tománek**

PoS Su31 **TEM and SFM Investigation of Single Walled Carbon Nanotubes Grown by CVD Between Microprinted Catalyst Islands**
G. Philipp, G. Gu, X. Wu, M. Burghard, A. Bittner and S. Roth

PoS Su32 **Non-Contact Scanning Force Microscopy Induced CVD: First Attempts Towards Contacting Nanotubes on an Insulating Substrate**
M. D. Croitoru, A. Höchst, W. Clauss, S. Roth, D. P. Kern

PoS Su33 **Direct Nano - Bridging of Carbon Nanotube Using Growth Barrier for Nanoelectronics: A Possible Mechanism of Selective Lateral Growth and Observation of Field Effect**
Yun-Hi Lee, Dong-Ho Kim, Yoon-Taek Jang, Chang-Woo Lee, Chang-Hoon Choi, **Gyu-Tae. Kim**, Eun-Kyu Kim, Byeong-Kwon Ju,Jae-Eun Lee, Young-Soo Hahn, Sang-Soo Yoon, Jin-Koog Shin, Sung-Tae Kim

PoS Su34 **Temperature Dependence of Field Effect Function of a Direct Bridged CNT Between Ferromagnetic Electrodes: Ni as Both Catalyst and Contact Electrode**
Dong-Ho Kim, Yun-Hi Lee, Chang-Woo Lee, Yoon-Taek Jang, Chang-Hoon Choi, **Gyu-Tae Kim**, Eun-Kyu Kim, Byeong-Kwon Ju, Jae-Eun Lee, Young-Soo Hahn, Sang-Soo Yoon, Jin-Koog Shin, Sung-Tae Kim

PoS Su35 **Computational Studies of Catalysed Nanotube Growth**
Kim Bolton and Arne Rosén

PoS Su36 **Formation Mechanism of Single-Wall Carbon Nanotubes and Single-Wall Carbon Nanohorns**
M. Yudasaka, Y. Kasuya, D. Kasuya, F. Kokai, K. Takahashi, S. Iijma

PoS Su37 **Coalescence of Fullerenes in Single-Walled Carbon Nanotubes**
Kaori Hirahara, Shunji Bandow, Masako Yudasaka, Kazutomo Suenaga and Sumio Iijima

Monday, July 23, 2001: Invited Talks

Mo1 A **Carbon Nanotube-Based Hybrid Materials**
David E. Luzzi

Mo1 B **Carbon Nanomaterials in Heterogeneous Catalysis**
R. Schlögl, G. Mestl, E. Sanchez, N. Maximova

Mo2 A **Controlling the Electronic Properties of Carbon Nanotube Bundles**
Philip G. Collins, Richard Martel, Phaedon Avouris

Mo2 B **When are Carbon Nanotubes Ballistic Conductors?**
Walt A. De Heer

Mo3 A **Recent Transport and STM Results on Carbon Nanotubes**
Cees Dekker

Mo3 B **Theoretical Study of the Quantum Conductance of Nanotube Structures: Defects, Junctions, and Peapods**
Steven G. Louie

Monday, July 23, 2001: Poster Presentations

PoS Mo1 **Multiwalled Carbon Nanotubes as Nanoscale Electronic Devices**
M. Ahlskog, R. Tarkiainen, L. Roschier, and P. Hakonen

PoS Mo2 **A Study on the Electrical Transport in and Between Single-Wall Carbon Nanotubes**
J. Appenzeller , H. Stahl , B. Lengeler, R. Martel , Ph. Avouris

PoS Mo3 **Electronic Transport in Multi - Walled Carbon Nanotubes**
M.R. Buitelaar, M. Iqbal, T.Nussbaumer, L. Fórró and C. Schönenberger

PoS Mo4 **Electronic Transport and Structure in Carbon Nanotube Junctions**
Hyoung Joon Choi, Jisoon Ihm, Young-Gui Yoon, Steven G. Louie, and Marvin L. Cohen

PoS Mo5 **Electronic Transport in Ultra-Clean Single-Walled Carbon Nanotubes**
M. S. Fuhrer, A. Bachtold, M. Forero, A. Zettl, Paul L. McEuen

PoS Mo6 **Multiwalled Carbon Nanotube: Luttinger Liquid or Not?**
R. Tarkiainen, M. Ahlskog, J. Penttil, L. Roschier, P. Hakonen, M. Paalanen, and E. Sonin

PoS Mo7 **Transport of annealed MWCNT and Its Application to Transistor Device**
Jaeuk Chu, Kwangseok Jeong, Eunju Bae and Wonbong Choi, Minho Yang, Seahn Song Hyoung Joon Choi, Jisoon Ihm, Young-Gui Yoon

PoS Mo8 **Conductance of Multi-Wall Carbon Nanotubes**
Anders Hansson , Magnus Paulsson, and Sven Stafström

PoS Mo9 **Anderson Localization in Metallic Carbon Nanotubes**
M. Hjort and S. Stafström

PoS Mo10 Barrier Formation in Electrical Contacts Between Metal and Multi-Wall Carbon Nanotube
A. Kanda , K. Tsukagoshi, Y. Ootuka, and Y. Aoyagi

PoS Mo11 Effects of a Perpendicular Magnetic Field on the Nanotube Conductivity
Alex Kleiner and Sebastian Eggert

PoS Mo12 Band Gap Modification by Circumferentially Perturbing Potentials in Carbon Nanotubes
Yong-Hyun Kim and K. J. Chang

PoS Mo13 Electrical Transport Properties in Multi-Wall Carbon Nanotube p-p Hetero-Junction
J.-O. Lee, H. Oh, J. -R. Kim, K.C. Kang, and J.J. Kim, J. Kim , J. W. Park, K.H.Yoo

PoS Mo14 Single Wall Nanotube Field-Effect Transistors and Logic Circuits
R. Martel, V. Derycke, C. Lavoie, P. Wong, and Ph. Avouris

PoS Mo15 Electronic Transport Behaviour in Carbon Nanotube Ropes
G. C. McIntosh, G. T. Kim and Y. W. Park

PoS Mo16 Wave-Vector Conservation and Electric Transport Through Crossed Carbon Nanotube
Takeshi Nakanishi and Tsuneya Ando

PoS Mo17 One-Dimensional Localization in Single-Wall Carbon Nanotubes
F. Nihey, T. Ichihashi, M. Yudasaka, and S. Iijima

PoS Mo18 Kondo Effect in Carbon Nanotube Quantum Dots
Jesper Nygård, David H. Cobden Und Poul Erik Lindelof

PoS Mo19 Electrical Transport in Nanotubes With Realistic Contacts: An ab-initio Study
J. J. Palacios, A. J. Perez-Jimenez, E. Louis, and J. A. Verges

PoS Mo20 Multiwalled-Carbon Nanotubes as Non-Ballistic Conductors
F. Triozon, A. Rubio, D. Mayou and **S. Roche**

PoS Mo21 Influence of Length on the Electrical Transport into Metallic, Semiconducting, and M-S Junction Carbon Nanotubes
Alain Rochefort, Massimiliano Di Ventra and Phaedon Avouris

PoS Mo22 Resonant Tunneling in Carbon Nanotubes in Presence of Two Tunneling Junctions
M. Thorwart, M. Grifoni, H.W. Ch. Postma, and C. Dekker

PoS Mo23 Real Space Imaging of Interfering Bloch Waves on Carbon Nanotubes at Room Temperature
A. Hassanien, P. Umek, A. Mrzel, M.Tokumoto and D. Mihailovic

PoS Mo24 New Opportunities Lead to New Roles for Science and Business
Silke Burkart, Silvester Schmidt

Monday, July 23, 2001: After Dinner Presentation

MoAD **Perspectives on the Role of Carbon Nanotube Research in the Worldwide Nanotechnolgy Initiative**
Mildred Dresselhaus

Tuesday, July 24, 2001: Invited Talks

Tu1 A **Novel Layered Nanomaterials: Controlled Synthesis, Electronic Properties and Applications**
Mauricio Terrones

Tu1 B **Optical Properties of Fullerene- and Non-Fullerene-Peapods**
H. Kataura, T. Kodama, K. Kikuchi, K. Hirahara, K. Suenaga, S. Iijima, W. Kraetschmer, S. Suzuki and Y. Achiba

Tu2 A **The Optical Properties and Electronic Structure of SWCNT: Empty, Stuffed or Surrounded by Dopants**
M. S. Golden, X. Liu, T. Pichler, M. Knupfer, J. Fink, D. Walters, M. J. Bronikowski, R. E. Smalley, H. Kataura, O. Jost, A. A. Gorbunov and W. Pompe

Tu2 B **Molecule/SWNT Interactions: Effects on Electronic and Phonon Properties**
Peter C. Eklund

Tu3 A **Chemistry of Single-Walled Carbon Nanotubes**
Robert C. Haddon

Tuesday, July 24, 2001: Poster Presentations

PoS Tu1 **Fluorinated Single-Wall Carbon Nanotubes**
A.V. Okotrub, N.F. Yudanov, L.G. Bulusheva, A.I. Romanenko

PoS Tu2 **Properties of Fluorinated Single-Walled Carbon Nanotubes as Derived From Density Functional Computations**
Holger F. Bettinger, Konstantin N. Kudin, Gustavo E. Scuseria

PoS Tu3 **SWNTs Modified by Selective Nanoparticle Attachment**
Y. Fan, S. Kooi, U. Schlecht, M. Burghard, K. Kern

PoS Tu4 **The Chemistry of Single Walled Carbon Nanotubes**
Michael Holzinger and Andreas Hirsch

PoS Tu5 **Theoretical Investigation on the Insertion of Li+ into Carbon Nanotubes**
Tapas Kar*, J. Pattanayak and S. Scheiner

PoS Tu6 **Electrochemical Modification of Carbon Nanotubes**
S. Kooi, Y. Fan, U. Schlecht, M. Burghard, K. Kern

PoS Tu7 **Electronic Structure of Pristine, Fullerene-Filled and Intercalated SWCNT From High Resolution EELS in Transmission**
X. Liu, T. Pichler, M. Knupfer, M. S. Golden, J. Fink, D. Walters, M. J. Bronikowski, R. E. Smalley, and H. Kataura

PoS Tu8 **Synthesis of Soluble Single-Walled Carbon Nanotube Derivatives**
E. Menna, F. Della Negra, M. Cavallaro, M. Maggini, G. Scorrano, M. Meneghetti, F. Paolucci, M. Battagliarin

PoS Tu9 **Nanoring Formation by Ring-Closure Reactions of Carbon Nanotubes**
M. Sano, A. Kamino, J. Okamura, S. Shinkai

PoS Tu10 **Reversible Water-Solubilization of Single-Walled Carbon Nanotubes by Polymer Wrapping**
Michael J. O'Connell, Peter Boul, Lars M. Ericson, Chad Huffman, Yuhuang Wang, Erik Haroz, Kevin D. Ausman, and Richard E. Smalley

PoS Tu11 **Raman Imaging of Chemically Modified Individual Carbon Nanotubes**
A. Mews, C. Jiang, T. Schuessler, F. Koberling, T. Basché, G. Philipp,M. Burghard

PoS Tu12 **Charge Transfer in Potassium Doped C_{60} Peapods From Resonance Raman Scattering**
T. Pichler, W. Planck, A. Grüneis, H. Kuzmany, H. Kataura, Y. Achiba

PoS Tu13 **Raman Studies of Alkali-Doping of SWNT**
J.-L. Sauvajol, N. Bendiab, A. Zahab, E. Anglaret

PoS Tu14 **Visible Emissions of Single-Walled Carbon Nanotubes Formed in Zeolite Crystals**
N. Nagasawa, I. Kudryashov , and Z. K. Tang

PoS Tu15 **Gas Adsorption Property of Single-Wall Carbon Nanohorns**
K. Murata, K. Kaneko, D. Kasuya, K. Takahashi, F. Kokai, **M. Yudasaka** , and S. Iijima

PoS Tu16 **Xenon Adsorption on the Outer Surface of Closed Ended SWNT Bundles**
S.Talapatra, N.Dolan and A.D.Migone

PoS Tu17 **STM Study of a Grain Boundary in Graphite**
P. Simonis, C. Goffaux, V. Meunier, L.P. Biro and P. A. Thiry

PoS Tu18 **Application of Partitioned Real-Space Density Functional Method to Field Evaporation From Carbon Nanotubes**
N. Nakaoka, K. Tada, and **K. Watanabe**

PoS Tu19 **Iron Catalyst Chemistry in High Pressure Carbon Monoxide Nanotube Reactor**
Carl D. Scott, **Pavel Nikolaev**, Alexander Povitsky, Chris Dateo, Tahir Gokcen, Richard E. Smalley

PoS Tu20 **Hydrogen Storage Mechanism in Single-Walled Carbon Nanotubes**
Seung Mi Lee, Young Hee Lee, Gotthard Seifert, and Thomas Frauenheim

PoS Tu21 **Tribo-Effects in Nanotubes**
Petr Král

Wednesday, July 25, 2001: Invited Talks

We1 A **Carbon Nanotube and Its Application to Nanoelectronics**
W.B. Choi[1], J.J. Kim[2], J.U. Chu[1], E.J. Bae[1], K.S. Chung[1]

We1 B **Carbon Nanostructures: Growth, Electron Emission, Interactions With Hydrogen**
Louis Schlapbach, Oliver Gröning, Pascal Ruffieux, Lars-Ola Nilsson, Patrick Sudan, Philipp Mauron, Christophe Emmenegger, Pierangelo Gröning, Andreas Züttel

We2 A **Inorganic Nanotubes and Inorganic Fullerene-Like Materials of Metal Dichalcogenides**
Reshef Tenne

We2 B **CVD Synthesis of Single Walled Carbon Nanotubes on Aerogel Supported Catalysts**
B. Zheng, Y. Li, M. Su and **J. Liu**

We3 A **Theoretical Studies of Quantum Transport, Pyro- and Piezo-Electric Effects and Lithium Intercalation**
J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, C. Roland, and Q. Zhao

We3 B **Carbon Nanotube Molecular Wires: Recent Progress in Synthesis, Characterization and Devices**
Hongjie Dai

Wednesday, July 25, 2001: Poster Presentations

PoS We1 **CVD Grown Carbon Nanotube Tips for Atomic Force Microscopy**
V. Barwich, R. Bennewitz, **A. Baratoff** and E. Meyer

PoS We2 **Symmetry Principles of Friction – Nanotubes**
Milan Damnjanovic, Tatjana Vukovic and Ivanka Milosevic

PoS We3 **Hollow Nanoparticles of WS_2 as Superior Solid Lubricant**
L. Rapoport, V. Leshzinsky, I. Lapsker, M. Lvovsky, Yu. Volovik, R. Rosentsveig, Y. Fedman and **R. Tenne**

PoS We4 **Scaling Laws for Van Der Waals Interaction of Hollow Nanoparticles**
U. S. Schwarz and S. A. Safran

PoS We5 **A New Hybrid Nanocomposite Formed by Intercalation of Multi-Walled Carbon Nanotubes into Epoxy Swelled Montmorillonite Clay**
Peter Butzloff, Nandika Anne D'Souza, Yi Sun

PoS We6 **Synthesis and Characterization of Single-Walled Carbon Nanotubes/Polymer Network Composites**
H. Goering, H.-E. Maneck, U. Knoll, S. Gajewski, K.-W. Brzezinka, R. Mach, H.-D. Klotz, A. Schönhals, J.F. Friedrich

PoS We7 **Carbon-Nanofibre-Filled Thermoplastic Composites**
Jan Sandler, Milo Shaffer, Jacek Nastalczyk, Christian Keun

PoS We8 **Electronic and Mechanical Properties of Hydrogen Functionalized Carbon Nanotubes**
Liu Yang, Richard Jaffe, Jie Han

PoS We9 **Simultaneous Determination of Inclusion Crystallography and Nanotube Conformation for a Sb_2O_3:SWNT Composite**
S. Friedrichs, R.R. Meyer, J. Sloan, A.I. Kirkland, J.L. Hutchison, M.L.H. Green

PoS We10 BN and B/N-Doped C Nanotubes: Synthesis, Structure, Properties and Applications
Dmitri Golberg and Yoshio Bando

PoS We11 Structural Stability and Electronic Structure of Boron Nanotubes
D. Ceresoli , E. Tosatti

PoS We12 BN Substituted Carbon Compounds: A Theoretical Study
Tapas Kar, J. Pattanayak and S. Scheiner

PoS We13 Vanadium Oxide Nanotubes as Cathode Materials in Rechargeable Lithium Batteries
Kristina Edström, Sara Nordlinder, Torbjörn Gustafsson, Jun Lu and Eva Olsson

PoS We14 Carbon Nanotube Based Composites as Electron Injection Layers in Organic Light Emitting Diodes
JN Coleman, P Fournet, A Drury, B Kilbride, HH Hoerhold* and WJ Blau

PoS We15 Systematic Study of Carbon Nanotubes Static Polarizabilities as a Function of Radius, Length and Helicity
M. Devel, Ch. Adessi

PoS We16 Field Enhancement Properties of Carbon Nanotubes
Ch. Adessi, **M. Devel**

PoS We17 Field Emission From Individual Carbon Nanotubes: Towards a High-Brightness Electron Source
N. De Jonge, M.W. Kreijveld, and **N.J. Van Druten**

PoS We18 MOCVD Approach to Aligned Isolated Carbon Nanotubes. Materials for Cold Cathode Field Emitters
J. J. Schneider, **J. Engstler**, G. Mueller, B. Guenther

PoS We19 Field-Dependent Secondary Electron Emission From MgO-Deposited Carbon Nanotubes
Jisoon Ihm, Youngmi Cho and Gunn Kim

PoS We20 Field Emission Energy Distribution for an Undergated Triode CNT-FED
Sunghwan Jin, Whikun Yi, **SeGi Yu**, Jungho Kang, Taewon Jeong, Jeonghee Lee, Jungna Heo, Yongsoo Choi, Wonseok Kim, Y.H. Lee, and J.M. Kim

PoS We21 Growth and Properties of CVD-Grown Carbon Nanotube Films
F. Rohmund, R.-E. Morjan, M. Sveningsson, O.A. Nerushev, A. Gromov, L.K.L. Falk, E.E.B. Campbell

PoS We22 Oxidation in Air of CCVD and Laser-Ablation Carbon Nanotubes
E. Hallberg, R. Bacsa, S. Rul, A. Peigney, **Ch. Laurent**

PoS We23 Scroll-to-Nanotube Transformation: The Zipper Mechanism
Savas Berber and **David Tománek**

PoS We24 Scrolls and Nested Structures in Multiwalled Carbon Nanotubes
Shekhar Subramoney, Gerry Lavin, Rodney Ruoff, David Tománek, Savas Berber

PoS We25 Transformation of Single-Wall Carbon Nanotube Ropes into Multiwall Carbon Nanotubes
Maria J. Lopez, Angel Rubio, Julio A. Alonso, Sylvie Bonnamy

PoS We26 Hydrogen Storage in Carbon Nanotubes: A Neutron Scattering Investigation
B. Renker , S. Lebedkin , H. Schober , M. Koza , M.M. Kappes

PoS We27 Application of Carbon Nanotubes to Energy Storages
Y. H. Lee, K. H. An, **S. M. Lee**, W. S. Kim, K. G. Jeon, Y. S. Park, J. M. Moon

PoS We28 Curvature and Hybridization Effects in Carbon Nanotubes
Alex Kleiner and **Sebastian Eggert**

PoS We29 Ab Initio Calculation of the Absorption and Energy-Loss Spectra of a Bundle of Carbon Nanotubes
A. G. Marinopoulos, Lucia Reining, Angel Rubio and Valerio Olevano

PoS We30 Plasmon Excitations in Isolated SWCNT
I. Milosevic, T. Vukovic, S. Dmitrovic, M. Damnjanovic

PoS We31 Dynamics of Low Energy Optical Excitations in SWNTs: Cooling of a Laser Heated Electron Gas and Non-Equilibrium Effects
G. Moos, R. Fasel and T. Hertel

PoS We32 Light Emission From Carbon Nanotubes
J.S Lauret, C. Delalande, **Ph. Roussignol**, A. Filoramo, J.N. Patillon, A.M. Bonnot, M. Chaumont, T. Fournier, L. Pontonnier, S. Roche, S. Landis

PoS We33 Transport and Magnetic Properties of Brominated Multiwall Carbon Nanotubes
A.I. Romanenko, A.V. Okotrub, Cheng Dong, Yongming NI, O.B. Anikeeva, L.G. Bulusheva, N.F. Yudanov

PoS We34 Nonlinear Optics of Intense Ultrashort Light Pulses in Carbon Nanotubes
G.Ya. Slepyan, A.A. Khrushchinskii, S.A. Maksimenko, V.P. Kalosha, and J. Herrmann

PoS We35 Adsorption Studies of Xenon on Carbon Nanohorns
A.J.Zambano,W.Mcmillin, **S.Talapatra**,G.Shaugnessey and A.D. Migone

PoS We36 Nanotube Sensors for the Detection of Failures Within Integrated Circuits
Glenn Wright, Marek Zgol, Susanna Keeton

PoS We37 Structural and Electronic Properties of a Carbon Nanotorus: Effects of Extended Vs Local Deformations
S.Y. Wu , L. Liu, and C.S. Jayanthi

PoS We38 Evaluation of the Mechanical Properties of Carbon Nanotubes and Nanofibres Under Hydrostatic Pressure by Laser-Raman-Spectroscopy
Milo Shaffer , Jan Sandler, Miguel Montes, Carole Cooper, Alexander Kalabushkin, Karl Schulte, Alan H. Windle, Robert J. Young

PoS We39 A Neutron Scattering Investigation of the Pressure-Induced Structural Changes and Low Frequency Excitations in SWNT Bundles
J.-L. Sauvajol, S. Rols and R. Almairac

PoS We40 Hydrogen Adsorption on Different types of Nanotubes
M. Ashraf Imam, and R.O. Loutfy

Abstracts Sunday

Su1 A 8.40-9.25

Single-Wall Graphite Sheets as Molecule Adsorption

Sumio Iijima

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It is quite natural that large specific surface areas of single graphene sheets such as single Wall carbon nanotubes(SWNT s) and single Wall carbon nanohorns (SWNHs) can be utilized for gas adsorption studies. In this talk I will describe various types of carbon materials in terms of their growth, atomic structures and their chemical modifications, and relate them to molecule adsorption. Firstly I will discuss encapsulation of fullerenes and metal-endohedral fullerenes into central hollows of SWNTs with emphasis of a one-dimensional ordering. The doping dynamics of fullerene molecules into SWNTs are quite useful for understanding adsorption process of gas species on graphite. This part of my talk includes double-Wall carbon nanotubes which we re formed upon heating fullerenes doped SWNTs. Secondly I like to speak about SWNHs in terms of technological importance of gas adsorption and selectivity beside other applications such as electron field emitters. The SWNHs are spherical particle of ~80nm in diameter whose surfaces are covered with tubular graphene layers with horn-shaped caps. The nano-horns are formed at room temperature without metal catalyst unlike SWNTs and consist of pure graphene layers. Taking advantages of large quantity production and high purity of SWNHs over SWNTs, we demonstrate that depending upon heat-treatment of SWNTs under an oxygen atmosphere the gas adsorption nature can be controlled, and a particular molecular size can be selected. Thirdly I will touch upon adsorption characteristic of processed SWNTs and SWNHs with large macro-molecules.

Su1 B 9.25-10.10

Root Growth Mechanism for Single-Wall Nanotubes

A. Loiseau[1], J. Gavillet[1], C. Journet[2], F. Willaime[3], F. Ducastelle[1] and J-C. Charlier[4]

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[3]Section de Recherches de Métallurgie Physique (SRMP),CEA/Saclay, 91191 Gif-sur-Yvette, France
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Carbon single-Wall nanotubes (C-SWNTs) can be produced by arc discharge, solar furnaces, which are high temperature processes, and catalytic methods which are medium temperature syntheses. In all cases, metallic catalysts are necessary for their formation. On the contrary, a route to the synthesis of boron nitride single-Wall nanotubes (BN-SWNTs) in gram quantities has been recently developped using a continuous CO_2 laser ablation reactor without the benefit of a catalyst [1]. In this conference we will show that in both cases the formation process, which can be deduced from minutious high resolution transmission electron microscopy studies, implies a root growth mechanism at the surface of a nanoparticle.

[1] R. S. Lee, J. Gavillet, M. Lamy de la Chapelle, A. Loiseau, J.-L. Cochon, D. Pigache, J. Thibault, F. Willaime, submitted to Phys. Rev B, Rapid Comm (2001).

Su2 A 10.30-11.15

Thermal Properties and Quantized Phonon Spectrum of Single-Walled Carbon Nanotubes

James Hone

California Institute of Technology, Pasadena, CA 91125, USA

We describe measurements of the specific heat and thermal conductivity of bundles of SWNTs and MWNTs. The temperature-dependent specific heat directly probes the phonon energy spectrum. The data provide direct evidence that the individual tubes' phonon spectrum is quantized due to their small radii. In addition, the specific heat is a sensitive probe of the mechanical coupling between neighboring tubes in SWNT ropes. The measured specific heat is consistent with a tube-tube coupling that is much weaker than would be expected from simple comparison to graphite. This weak coupling has implications for both the mechanical and thermal properties of SWNT bundles. The thermal conductivity of both SWNTs and MWNTs is large, and also provides evidence for a quantized phonon spectrum.

Su2 B 11.15-12.00

Disorder and Pressure Effect on the Physical Properties of Carbon Nanotubes

Laszló Fórró

Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We have studied the role of disorder/impurities introduced by: i) the ferromagnetic catalytic particles; ii) fast electron irradiation; and iii). chemical manipulations. Their effect on the electronic, magnetic and mechanical properties of both for SWNTs and MWNTs will be reported.
Hydrostatic pressure changes the overlap integrals, electronic correlations and eventually the structure of the SWNTs. Its effect on the electrical resistivity and thermoelectric power will be discussed.

Work performed in collaboration with R. Gaál, N. Barisic, S. Garaj, A. Kis, L. Thien-Nga, J.-P. Salvetat, J.-M. Bonard

Su3 A 13.30-14.15

Transport in Carbon Nanotubes

M. Bockrath, W. Liang, D. Bozovoc, J. Hafner, C. M. Lieber, M. Tinkham, H. Park

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I will discuss our recent transport measurements of individual single-walled carbon nanotubes that have low ohmic contacts. The resistance of these samples approaches 6.5 kOhm -- the minimum possible resistance for nanotubes, which have two spin-degenerate propagating modes at the Fermi level. These samples show the influence of standing waves on the electron transport, leading to Fabry-Perot-like resonances as the Fermi wavelength in the nanotube is varied via an applied gate voltage. Furthermore, we have characterized defects in individual metallic single-walled carbon nanotubes by transport measurements and scanned gate microscopy. A significant fraction of metallic nanotubes exhibits gate-voltage dependent resistance at room temperature. Scanned gate measurements reveal that this behavior originates from resonant electron scattering by defects in the nanotubes. The overall behavior is in agreement with theoretical calculations of scattering from various simple defects. An intra-tube quantum-dot device formed by two defects illustrates the potential molecular electronics applications of these defects.

Su3 B 14.15-15.00

Spin Transport and Coulomb Blockade in Nanotubes

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[2] *Imperial College London, UK*

Coulomb interactions among conduction electrons play a major role in the transport behavior of SWNTs and MWNTs. While in SWNTs ballistic transport prevails and causes Luttinger liquid behavior, in MWNTs one has a diffusive system with nevertheless important manifestations of interactions. This talk describes two hallmarks of interaction physics in nanotubes, namely (1) spin transport and spin-charge separation in SWNTs, and (2) the recently observed zero-bias power law anomaly in the tunneling density of states in MWNTs, The latter is caused by Coulomb blockade in terms of an "exponentiated" Altshuler Aronov correction.

PoS Su1 15.30-18.30

Qualitative and Quantitative Assessment of the SWNT Produced by the Controlled Catalytic Production Before and After Purification

F. Pompeo, L. Balzano, H. Barraza, J. E. Herrera, E. O'Rear, S. Dahl[1], W.E. Alvarez, **D. E. Resasco**

University of Oklahoma
[1] Haldor Topsoe

The quantification of the SWNT yield and the evaluation of their chemical characteristics are essential components in the development of a production process. In this particular study, the SWNT were produced by vapor-phase disproportionation of CO over a heterogeneous catalyst. Temperature programmed oxidation has been used to determine the total carbon yield as well as the selectivity to SWNT. The results of this quantitative method were corroborated by Raman and TEM/SEM analysis. After the SWNT production, the materials were subjected to purification steps that involve attack of the catalyst support and metals with a combination of basic and acid solutions. This process results in a different degree of functionalization of the tubes. The characterization of the chemical nature of the resulting functional groups was conducted by XPS and FTIR. To quantify the density of functional groups a combination of TPD-TPO and XPS was employed. The response of the tubes prepared by the catalytic method to the basic/acid attacks was compared to those of tubes prepared by other methods (arc discharge and laser ablation). Also, the structure of these tubes (bundle diameter, tube diameter, tube length), as measured by AFM, TEM and Raman, was compared to those commercially available.

PoS Su2 15.30-18.30

Room Temperature Growth of Single Wall Coiled Carbon Nanotubes and Y-Branches

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The growth of carbon nanotubes from fullerene fragments produced by catalytic decomposition in the presence of transition metals at about 450 °C was investigated. The nanotubes are grown by vapour deposition on highly oriented pyrolytic graphite (HOPG) at room temperature. No further purification or manipulation is necessary for investigations by scanning tunneling microscopy. The templating effect of the substrate is assumed to be an important growth condition. No tubes were found on Au(111) or mica surfaces. Individual tubes as well as raft like structures of multiwalled tubes and bundles of single walled tubes were on HOPG. Several cases of Y- branching of single Wall carbon nanotubes were observed with an angle of approximately 120° between the branches and a branch diameter of about 1.6 nm. Tightly wound "telephone cable-like" coils were found too.

PoS Su3 15.30-18.30

Defects in the Catalytic Multiwall Carbon Nanotubes

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Thermal decomposition of hydrocarbons on the metal catalyst yields bent and curved multiwall nanotubes, the layers of which are often wavy and segmented. Such structural distinguishes from the typical arc-produced multiwall carbon nanotubes can cause the difference in the electronic structure for two tube kinds. To check it the methods of X-ray emission and X-photoelectron spectroscopy were used. Comparison between measured spectra detected that, actually, the C Kα spectrum of catalytic nanotubes is characterized by enhanced density of π-occupied states and the C 1s line of this sample is expanded toward both lower and higher binding energy regions. To reveal what type of structural defects can explain the experimental data the tubular models incorporated pentagon-heptagon pairs, sp^3-hybridized atoms, and incomplete bonds were calculated using quantum-chemical program AM1. Carbon Kα and 1s lines were found to be practically unaffected by inserting pentagon and heptagon into the hexagonal network on diametrically opposite sides of tube. The adjacent position of defect pair gives the better while still not adequate fit to the experiment. However, the interlayer linkages and holes in the carbon network may provide the expected spectral changes.

PoS Su4 15.30-18.30

Investigation of the Growth Mechanism of Vertically Aligned Carbon Nanotubes Using High Resolution Electron Microscopy

C. Ducati [1], M. Chhowalla[1], K.B.K. Teo[1], I. Alexandrou[1], N.L. Rupesinghe[1], G.A.J. Amaratunga[1], J. Robertson[1], W.I. Milne[1], A. Papworth[2], C.J. Kiely[2]

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The growth mechanism of carbon nanotubes from solid-phase catalysts in hydrocarbon atmosphere can be described as a sequence of dissolution and diffusion of atomic carbon into a metal particle, formation of a metastable carbide, precipitation of a stable graphite phase forming the nanotube walls. Vertically aligned carbon nanotubes (VACNTs) have been grown by direct current plasma enhanced chemical vapour deposition (DC PECVD) on a nickel catalytic layer. The CNT film properties, such as average tube diameter, growth rate and areal density, are controlled by the initial thickness of the metal layer. The alignment of the tubes depends on the electric field applied during deposition. VACNTs have been characterised by high resolution electron microscopy (HREM) and scanning transmission electron microscopy (STEM) in order to gain an insight on the role of the catalyst particle in the tip-growth process. Direct evidence of metastable MexC phases that promote the segregation of carbon from the catalyst particle is reported. A detailed study on the growth of VACNTs will be presented. A model similar to that of Baker and Harris [1] is proposed to explain the growth mechanism of VACNTs.
[1] R.T.K. Baker, P.S. Harris, in 'Chemistry and Physics of Carbon' ed. P.L. Walker and P.A. Tower (Dekker, New York - 1978).

PoS Su5 15.30-18.30

Isotope Effects of CH_4 in Synthesis of Single-Walled and Multi-Walled Carbon Nanotube by Thermal Chemical Vapor Deposition

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We did the control composition of single Wall carbon nanotube (SWCNT) and aligned multi Wall carbon nanotube (MWCNT) on Si substrate from argon and methane as a carbon source by thermal chemical vapor deposition method. We used three kinds of CH_4 in the different isotope ratio. One is a natural abundance isotope ratio which composed of 98.9 % $^{12}CH_4$ and 1.1 % $^{13}CH_4$. The others are ^{12}C and ^{13}C enrichment of stable isotope CH_4 gas by cryogenic distillation of a natural abundance CH_4. The isotope enriching purity is 99.95 % for ^{12}C, and 99 % for ^{13}C. At first, we used CH_4 which is a natural abundance isotope ratio as a carbon source. We have fabricated SWCNT using a catalyst consisting of Fe or Co or Ni oxide with Mo oxide supported Al_2O_3 particles on Si substrate. SWCNT were grown at 900°C. Its diameter is 0.5 - 1.2 nm. And we have fabricated MWCNT. The metal of Pd or Fe or Co or Ni was utilized by thermal evaporation method. MWCNT were grown at 1100 - 1200°C.Its diameter is 150 - 200 nm. Second, [1] do similar experiments using isotope CH_4 ($^{12}CH_4$, $^{13}CH_4$) as raw materials. We report results of spectrum shift of IR and Raman. [1] Jing Kong, Hyongsok T.soh, Alan M.Cassell, Calvin F.Quake & Hongjie Dai.,Nature, 395(1998), 878-881

PoS Su6 15.30-18.30

Optical Absorption Study of Rate-Limiting Processes in the Laser Evaporation Synthesis of Single-Wall Carbon Nanotubes

O. Jost[1], A.A. Gorbunov[1], W. Pompe[1], X. Liu[2], M.S. Golden[2], and J. Fink[2]

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Optical absorption spectroscopy is known to offer an express, bulk-sensitive measure of the relative single-Wall carbon nanotube (SWCNT) yield in as-produced material [1,2]. Consequently, we performed a systematic study of synthesis parameters in the furnace-based laser evaporation synthesis of SWCNT including variations of the gas-type, gas-pressure and furnace temperature. In our contribution, we present selected results dealing with the determination of a number of rate-limiting processes. A total of four such rate-limiting processes could be found, two of them being not only rate-limiting but covering all the relevant gas-type and gas-pressure dependencies of the SWCNT formation. Two condensed-state-based thermally activated processes with their activation energies could also be determined. The results allow the derivation of a self-consistent flow-chart describing the proccesses taking place in the formation of SWCNT. This work was supported in part by the DFG (PO392/10-2 & FI439/8-2) and the EC (FET-NID initiative, project IST-10593-SATURN). [1] O. Jost et al., Appl. Phys. Lett. 75, 2217 (1999) [2] O. Jost et al., Chem. Phys. Lett., in press.

PoS Su7 15.30-18.30

Formation of Single- and Double-Walled Carbon Nanotubes by a CVD Method

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[2] *NUMAT, Department of Subatomic and Radiation Physics, Ghent University, Proeftuinstraat 86, B-9000 Gent, Belgium*
[3] *LPST, UMR CNRS 5477, Université Paul-Sabatier, 31062 Toulouse cedex 4, France*

The reduction in H_2-CH_4 atmosphere of oxide solid solutions containing transition metal cations produces metal (Fe, Co, Ni) or alloy particles small enough to catalyze the formation of SWNTs and thin MWNTs (mostly 2, 3 walls). In some cases the CNTs can be extracted by dissolution of the oxide and metal in dilute HCl. The composite powders and the extracted samples are studied by several techniques including scanning and transmission electron microscopy, Raman spectroscopy, ^{57}Fe Mössbauer spectroscopy and a macroscopical method involving specific surface area measurements and elemental carbon analysis. The influence of several synthesis parameters (metal content, reduction temperature, CH_4 content) on the formation of CNTs and undesirable species (poorly ordered carbon, nanocapsules) will be discussed. Several mechanisms are thought to be active for the formation of CNTs. In particular, it is shown that the second wall can grow inside the first one but that subsequent ones are formed outside. It is also possible that under given experimental conditions, the smallest (< 2 nm) catalyst particles preferably produce double-walled nanotubes rather than SWNTs.

PoS Su8 15.30-18.30

Growth Mechanism of Bamboo-Shaped Carbon Nanotubes Using Thermal Chemical Vapor Deposition

C. J. Lee[1], T. J. Lee[1], S. C. Lyu [1], and J. E. Yoo[2]

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Since the first observation of carbon nanotubes (CNTs), extensive researches have focused on the synthesis of CNTs with high purity. Various synthetic methods such as arc discharge, laser vaporization, pyrolysis, and plasma-enhanced and thermal chemical vapor deposition (CVD) were employed. Despite great progress in the growth of CNTs, the growth mechanism has still not been completely understood. Given the different synthetic techniques, it is likely that a variety of mechanisms play a role in the growth of CNTs. Two growth models, i. e. base growth and tip growth models, were proposed for the catalytic growth of carbon nanotubes. In this works, we found no encapsulated catalytic particles at the closed tip from the bamboo-shaped CNTs grown by thermal CVD of acetylene (C_2H_2) at temperatures range 750-950 °C. Moreover, CNTs have compartment curvatures toward the tip. Based on the experimental results, we suggest a base growth model for the bamboo-shaped CNTs grown using thermal CVD method.

PoS Su9 15.30-18.30

Multiwall Carbon Nanotubes Grown on Metallic Substrates

F. Kreupl, A. Graham, E. Unger, **M. Liebau**, W. Hönlein

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Chemical vapour deposition is a well-known technique used throughout the semiconductor industry and is therefore the method of choice when it comes to an implementation of carbon nanotubes (CNTs) in a process flow. Whereas CNTs grown on oxidic substrates are well established, much less efforts and success has been reported on CNTs grown on metallic surfaces. This is where our recent studies are focusing on. In order to exploit the high electrical performance of CNTs, they have to be connected at both sides with highly conductive, i. e. metallic contacts. Besides the quality of the grown CNTs it is also very important that they can be grown on metallic surfaces giving inherently a good contact resistance due to the close contact to almost all layers of a multi-Wall CNT. We will report on the compatibility of various catalyst/metallic substrate combinations, which are producing multi-Wall CNTs of high quality.

PoS Su10 15.30-18.30

Single Carbon Nanotube Raman Spectroscopy

M.S. Dresselhaus[1], Ado Jorio[1], G. Dresselhaus[1], and R. Saito[2]

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The very sharp one-dimensional density of electronic states in small diameter single Wall carbon nanotubes and the strong electron-phonon coupling allow observation of the Raman spectra from one single Wall carbon nanotube when the incident or scattered photon is in resonance with an interband transition E_{ii} between singularities in the joint density of states between the valence and conduction bands. Observation of the Raman spectra of the radial breathing mode from an individual nanotube is used to provide a definitive identification of its structure through determination of the *(n,m)* indices. Variations of this basic method for different cases are discussed. This information is further used to determine to high resolution the profile of the joint density of states near a van Hove singularity. Because of the high sensitivity of the electronic, transport, vibrational and other nanotube properties to the structural *(n,m)* indices, this non-destructive, readily available characterization technique is expected to have a significant impact on current basic research on carbon nanotubes.

PoS Su11 15.30-18.30

Comparison of Diameter Distribution of SWCNT Bundles as Analyzed by Scanning Probe Microscopy and by Raman Measurements

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Due to the fabrication process SWCNTs appear mostly as bundles of varying diameters. It has been reported that the use of a strong solvent like DMF (dimethylformamide) in combination with sonication disentangles the nanotube ropes and thus provides individual SWCNTs. We analyzed the distribution of bundle diameter by Raman measurements and by SPM methods before and after sonication. A high dilution of SWCNT bundles and an consequent low area density allowed to get approximate statistics of the diameter distribution of the SWCNT bundles by SPM measurements. As a result of the experiments there were still bundles. Further dilution and sonication did not dissolve these bundles. Work is supported by the FWF projects P12924 and P14146 and the TMR Research Network 'FUNCARS' (HPRN-CT1999-00011) from the EU. T.P. thanks the ÖAW for funding.

PoS Su12 15.30-18.30

Accurate Density Functional Calculations of Phonons in Carbon Nanotubes

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The phonon dispersion relations of armchair and zigzag single-Wall carbon nanotubes are calculated using an all electron ab-initio density-functional method.[1] The behavior of the characteristic phonon branches, such as the radial breathing mode, twistons, the high-frequency optic modes and their dependence on the radius and the chirality are studied. The resulting spectra are in very good agreement with those obtained by the zone-folding method. We also present accurate force constants for isolated graphene sheets, which reproduce the experimental data with few percent accuracy. These force constants can be used for the study of the phonon dispersion relations of chiral tubes which are not directly tractable by first principle methods.
[1] G. Kresse, and J. Joubert, Phys. Rev. B 59, 1758 (1999).

PoS Su13 15.30-18.30

High Volume Production of Vapor Grown Carbon Nanofibers

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The serendipitous discovery of carbon nanotubes one decade ago has led to a new boost in carbon nanofiber technology. The structural perfection of this type of tubular graphitic carbon quickly revealed unexpected physical and chemical properties, which led to new visions and concepts in material science. As described in a great many deal of papers and patents tubular graphitic carbon might be introduced to a wide field of technical applications, like ultra light fiber reinforced composites, both with metals and plastics, in pastes as lubricant, electric or thermal conductor, in advanced coatings and as storage medium for hydrogen as well. So far so good, if there would not be the basic problem of production on a scale satisfying the demand for practical field tests at reasonable raw material costs. Though not yet fully understood in all detail, the catalytic activity of the iron group metals Fe, Co and Ni, respectively, being responsible for nanotube formation is well known and documented. Following this principle, we have developed a simple and cost effective CVD methodology yielding substantial amounts of nano fiber material in quantities between 50 and 200 grams per experiment in a pilot reactor unit. The wide range of yields is determined by the material quality finally obtained. As a rule of thumb it might be stated, that, the thinner the fibers and narrower the diameter distribution the lower the yield. As will be presented, the fiber diameters can be predetermined within a relatively small range, starting at 50 nm up to thick pyrocarbon coated fibers of several hundreds of nano meters. Structural features with respect to potential applications will be outlined.

PoS Su14 15.30-18.30

Length Measurements and Dispersion of Isolated Single-Wall Carbon

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Nanotube length and effects of subsequent purification are important with respect to the critical length and stress transfer issues in nanotube-based composites. This work focuses on the length of single Wall carbon nanotubes (SWNTs) produced by the pulsed laser vaporization technique, and effects of processing (purification, sonication) on it. Nanotube length was measured by AFM on pristine nanotube specimens as well as after sonication. In each case great care was taken to measure individual nanotubes, rather than bundles. Pristine nanotubes were collected on quartz substrates placed directly in the laser oven and exposed for 0.5 s. Their length is in excess of 20 micrometer, and their location and size distribution allowed us to conclude that nanotubes form very close to the target and continue to grow and bundle up in collisions as they travel away from it. Several nanotube specimens from various sources were deposited on silicon after extensive sonication. Nanotubes vary in length from 250 to 500 nm, which confirms that sonication cuts them. Issues of nanotube solubilization will also be discussed.

PoS Su15 15.30-18.30

Identification and Properties of 4Å Smallest Carbon Nanotubes

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The smallest carbon nanotube that remains stable energetically has diameter of 4A. We have produced such nanotubes employing an arc-discharge technique in hydrogen atmosphere and have identified them with high-resolution electron microscopy aided with extensive image simulations. Since the 4A nanotube gives rise to only very weak contrast, great caution must be exercised in establishing the identification. When the 4A nanotube resides inside a multiwalled carbon nanotube, the electron microscope image contrast bears clear signature of its presence, which is indicated by the fading image contrast towards the center of the nanotube. The electron microscopic imaging of single-walled carbon nanotubes of 4A diameter will also be discussed.

PoS Su16 15.30-18.30

Highly Selective Catalyst for Synthesis of SWNT by CO Disproportionation

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University of Oklahoma

The synthesis of single-walled carbon nanotubes (SWNT) by catalytic disproportionation of CO has been systematically investigated. A series of characterization techniques including Raman spectroscopy, TEM and TPO have been employed to characterize the carbon nanotubes. Among a many catalyst formulations investigated, a bimetallic Co-Mo catalyst has been found to be the most effective. A synergistic effect between Co and Mo has been observed. When both metals are simultaneously present, particularly when Mo is in excess, the catalyst is very effective. To understand this synergistic effect, X-ray absorption (EXAFS/XANES), FTIR, and UV/VIS spectroscopies have been used to characterize the state of Co and Mo on the catalysts before and after the production of SWNT. The selectivity of the Co-Mo catalysts towards SWNT production by CO disproportionation strongly depends on the stabilization of Co(II) species before the formation of SWNT begins. This stabilization results from an interaction with Mo and is only effective at low Co/Mo ratios. Under reaction conditions, the Mo oxide species are converted into Mo carbide, thus breaking the interaction and releasing the metallic Co in a state of high dispersion, which is responsible for the production of SWNT.

PoS Su17 15.30-18.30

Cost-Effective Controlled Production of Single-Walled Nanotubes

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University of Oklahoma

The rate of discovery of new and exciting properties of SWNT has yet to slacken. However, the development of commercial applications will remain a dream as long they are made by the laboratory methods available today. The full realization of the technological potential of nanotubes is contingent upon the development of industrial- scale synthesis. Applications such as SWNT-reinforced composites will never be realized as long as nanotubes are produced at rates of no more than grams per hour; an important step in advancing this technology is the development of techniques to produce tons of nanotubes per year. We have developed a "controlled production" method of SWNT. This term implies the ability to control the selectivity towards SWNT by changing catalyst formulations and operating conditions, combined with an effective purification strategy and a quantitative determination of the SWNT obtained. The use of heterogeneous catalysts allowed us to tailor the material in such a way that selectivity and yield are maximized. The method employed involves the disproportionation of CO at moderate pressure and temperature, which result in a scalable, cost-effective process. Optimal reaction conditions including temperature, pressures, gas-space velocities, catalyst composition and pre-treatments, as well as purification methods, will be reported.

PoS Su18 15.30-18.30

Gas Phase Synthesis of SWNT in an Atmospheric Pressure Plasma Jet

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We will present a new method for producing single Wall nanotubes (SWNT), wherein a gaseous mixture of argon, ethylene and ferrocene is passed through an atmospheric plasma. The plasma dissociates the molecules, and in the exhaust of the plasma flame, the atoms recombine to form SWNT, which are deposited downstream. Scanning electron microscopy (SEM), high resolution transmission electron microscopy (HR-TEM) and Raman spectroscopy were used to study samples taken from these deposits. The analyses indicate that the deposits are made up of SWNT, with diameters ranging from 1 to 1.5 nm.

PoS Su19 15.30-18.30

Nano-EELS Diagnoses of Hybrid Nanotubes, Nanocoils, and Nanocables

K. Suenaga

JST

Since the discovery of pure carbon nanotubes, researches for similar nanostructures involving non-carbon elements have been stimulated. The predicted electronic properties of these multi-element nanotubes are variable and essentially determinable by their chemical composition. Therefore the controlled production of hetero-junctions of such nanotubes can lead to the creation of a nanometer scale device with tailored electronic properties. A characterization tool with high spatial resolution is indispensable for the successful realization of such devices with anticipated geometry. Spatially resolved electron energy loss spectroscopy (EELS) is quite well-suited to such kinds of analysis: using an incident probe generated by a scanning transmission electron microscope (STEM), one is able to simultaneously perform elemental mapping and chemical state assignment at a sub-nanometer spatial resolution. Examples of hybrid nano-structures such as nanocoils, nanocables and B-C-N nanotubes those are promising candidates for nano-structured electronic devices, will be presented.

PoS Su20 15.30-18.30

Electron Beam Identification and Machining of Novel Hybrid Nanotubular Structures

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Nowadays can be considered as the nanotechnology era where materials at the nanometer scale (e.g. nanotubes), which present high potential properties, are being produced and investigated. The hollow structure of the nanotubes can be used as moulds for creating new nanostructures (e.g. nanowires), to encapsulate molecules as C_{60} or C_{82}@Gd and to store gas. The carbon nanotubes also can be doped with different elements as halides, B/N, to produce batteries or to get new nanodevices. However the identification of such complex B-C-N structures or SWNT@C_{82}@Gd requires accurate nanometre-scale analysis which is available in high-resolution imaging and electron microscpe. Carbon nanotubes containing nitrogen and nanocapsules regularly distributed along the tube axis, have been produced by pyrolysing camphor in the presence of nitrogen and ammonia. Spatially resolved electron energy-loss spectroscopic (EELS) analysis reveals that N_2 gas is encapsulated within the nanocapsules. The well-graphitized walls can be punctured by electron irradiation, thus partly releasing N_2, accompanied by the formation of amorphous CN_x island, as demonstrated by dynamic recording and analysis of time-resolved EELS sequences. Such local in-situ electron beam nanomachining and nanoanalysis provide a method for creating new classes of nanodevices.

PoS Su21 15.30-18.30

Polymer Forms of Single Wall Nanotubes

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A number of high-pressure-high-temperature structures of the SWNT structures are considered. Mechanism of polymerization for both doubly crossed (n,m) nanotubes and two parallel (n,n) and (n,0) SWNT's by means of cycloaddition process is discussed. Coupling of two neighbor nanotubes is energetically favorably under the "zipper" scheme. After readjustments of (2+2) cycloaddition of some atom pairs, step by step polymerization takes place along line between the tubes. Role of hydrogenation in the process of coupling and depolymerization of SWNT is discussed. The "zipper" mechanism is used to explain the following: 1) formation of zeolite structures [1], 2) transformation of molecular coupled nanotube rope into graphite needle under high pressure treatment [2]; 3) formation of double diameter nanotubes under high temperature and light atom flow treatment [3]. We have modeled some examples of polymer SWNT rope transformations using (n,n) and (n,0) carbon nanotubes with n=5-12. New nanotube polymer crystals are computed by using molecular mechanics [1] and a generalized tight-binding molecular-dynamic (GTBMD) method [4]. Energetic characteristics show high stability for all these structures. Furthermore, electronic band structures of such SWNT polymers show changing of electronic properties of original SWNT ropes from narrow semiconductor to dielectric: (12,12) NT structure with (2+2) cycloaddition [sp^3/sp^2 =1/4]; semiconductor crystals of (6,6) NT structure with (2+2) cycloaddition [sp^3/sp^2 =1], and (9,0) NT structure with (2+4) cycloaddition [sp^3/sp^2 =1/2]; high dielectric gap crystals of (6, 0) and (6, 6) NT structures with all sp^3 atoms. Some of considered structures have good agreement with experiments [3, 5]. This work was supported by "Atomic Clusters and Fullerenes" Russian Government Program, Russian Fundamental Fund of Investigation and NSF. [1] L.A. Chernozatonskii. Chem.Phys.Lett. 297 (1998) 257. [2] E.D. Obraztsova et al. in Elecrtonic Properties of Novel Materials. Proc. WINTERSCHOOL'99, Kirchberg. AIP Conf.Proc.486, N.Y. 1999. [3] P. Nikolaev, et al. Chem.Phys.Lett. 266 (1998) 322; S. Bonnamy et al. Proc. Carbon Conf., Tokyo, Nov.1998. [4] M. Menon, E.Richter, K.R.Subbaswamy, Phys.Rev. B 57 (1998) 4063. [5] M. Popov, M. Kyotani, Y. Koga et al. Phys. Rev. B (2001, in press)

PoS Su22 15.30-18.30

Excitonic-Insulating States in Carbon Nanotubes

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It has been demonstrated [1] that a long-lived spin accumulation can be injected into carbon nanotubes (CN's). Motivated by this experimental result, we theoretically consider a charge-neutral semiconducting CN where this spin accumulation corresponds to a quasi-equilibrium density of electrons and holes (in the lowest conduction and highest valence band, respectively) of the same spin direction. In mean-field theory, such a "spin-doped" (and, at first sight, conducting) system is unstable with respect to condensation of spin-triplet excitons, which are bound by the attractive electron-hole Coulomb interaction. The resulting ground state does not conduct and is called: "excitonic insulator". Taking into account a screened Coulomb interaction, we calculate the quasiparticle dispersion and find a gap (different from and not to be confused with the band gap of the intrinsically semiconducting CN) which decreases when the amount of spin (and hence electron-hole pair) doping is increased, but, suprisingly, does not vanish in the high-density regime, where the single-particle dispersion is almost linear and backscattering is strongly suppressed --- as in metallic CN's. In the latter regime, we discuss the validity and significance of our mean-field approximation by comparison with the Tomonaga-Luttinger liquid theory. [1] Tsukagoshi *et al*, Nature **401**, 572-574 (1999).

PoS Su23 15.30-18.30

Interwall Interaction and Charge Redistribution in Double-Wall Carbon Nanotubes

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Double-Wall carbon nanotubes (DWCNTs) are attracting increasing interest due to their spontaneous formation from single-Wall nanotubes filled with fullerenes under electron irradiation. Early theoretical studies have focused on the stability [1] and electronic structure [2] of selected DWCNTs. Here we report the first theoretical study of the charge distribution and electronic potential profiles of DWCNTs. Our self-consistent density functional calculations indicate a significant charge redistribution in nanotubes sandwiched in-between graphene sheets, and in double-Wall nanotubes. We find the net charge transfer to involve not only π-electrons in the system, but more importantly a new inter-Wall state, which is reminiscent of the interlayer state of graphite [3]. Our results elucidate the charge transfer trends and the common origin of the inter-Wall and inter-layer states. We also discuss how the modified charge density near the Fermi level affects Scanning Tunneling Microscopy images and the conductivity of multi-Wall nanotubes. This work was performed under the management of Frontier Carbon Technology supported by NEDO. [1] J.-C. Charlier and J.-P. Michenaud, Phys. Rev. Lett. 70, 1858 (1993). [2] Y. K. Kwon and D. Tománek, Phys. Rev. B58, R16001 (1998). [3] N.A.W. Holzwarth, S.G. Louie, and S. Rabii, Phys. Rev. B26, 5382 (1982), and references therein.

PoS Su24 15.30-18.30

A Density Functional Theory Study of Single Wall Nanotubes

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In our continuing efforts to design multi-functional materials with tailored properties we report a density functional theory study of single Wall carbon nanotubes with different diameters and chiralities. Carbon nanotubes are modeled as either one-dimensional or three-dimensional periodic systems in the simulations, corresponding to an isolated tube or a rope. Calculated structural and physical properties of carbon nanotubes and related systems will be discussed, in comparison with other theoretical work and experimental data.

PoS Su25 15.30-18.30

Quantum Interferences in Carbon Nanotubes

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The role of backscattering is scrutinized in doped semiconducting carbon nanotubes and in multi-wallled tubules. By computing the participation ratio in several systems, the quantum correction to the Bloch-Boltzmann conductivity together with localization charateristics are shown to strongly depend on the position of the chemical potential.

PoS Su26 15.30-18.30

Boron Nanotubes: A Theoretical Study

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A hexagonal layer of boron is now of high interest due to superconductivity with high transition temperature observed in MgB_2 in which boron atoms form graphitic layers. Accordingly, a formation of nanotubes from boron atoms is an interesting issue to be studied in detail. We will discuss the energetics and the electronic properties of boron nanotubes studied in the framework of the density-functional theory.

PoS Su27 15.30-18.30

On the Stability and Formation of Nanotubes

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On the basis of Density-Functional based tight-binding calculations a model explaining the stability pf single-Wall and multi-Wall carbon and non-carbon nanotubes is derived. The energetic competition between single-layer and multilayer sheets the corresponding single Wall and multi-Wall nanotubes is discussed. It is demonstrated how the energetics of a contious bending of flat sheets to tubular structures may serve as a possible path to the tube formation. Finally, it is shown how the bending barrier may be reduced by the presence of transition metals, as catalysts for tube formation.

PoS Su28 15.30-18.30

Linear Electrodynamics of Carbon Nanotubes

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Electronic and electromagnetic properties of carbon nanotubes (CNs) are considered in the microwave, the infrared and the visible regimes. Contribution comprises our recent results on linear electrodynamics of CNs [1-3]. Microscopic consideration of a CN's conductivity is undertaken both in the semi-classical approximation and on the basis of a rigorous quantum-mechanical model. Analytical expressions for the dynamic conductivity are derived and numerical results for different types of CNs are presented. Effective boundary conditions for the electromagnetic field and the electrostatic potential in CNs are stated on the nanotube surface providing thereby the most appropriate tool for solving electrodynamic problems involving CNs. The existence of surface TM-waves is pointed out and frequency ranges are shown to exist wherein these waves can propagate to distances essentially exceeding the CN length. That allows the concept of nanotubes as nanowaveguides. A composite medium comprising electrically small CNs dispersed in some host material is also considered. A homogenization procedure for such composites and some optical properties of them are discussed. [1] A. Lakhtakia, et al., Carbon 36, 1833 (1998). [2] G. Ya. Slepyan, et al., Phys. Rev. B57, 9485 (1998); B60, 17136 (1999). [3] S. A. Maksimenko and G. Ya. Slepyan, in "Electromagnetic Fields in Unconventional Structures and Materials", Ed. by: O.N. Singh and A.Lakhtakia, Wiley & Sons, New York 2000, pp. 217-255.

PoS Su29 15.30-18.30

Broken Symmetry, Boundary Conditions, and Band Gap Oscillations in Finite Single-Wall Carbon Nanotubes

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University of Lousiville

The interplay between the broken symmetry and the boundary conditions alters profoundly the electronic properties of carbon single-Wall (SW) nanotubes (NTs) of finite-lengths. For NTs *(p,q)* characterized by $p=k+l$, $q=k-l$, $0 \le l \le k$, and $k=1,2,\ldots$, the HOMO-LUMO gaps for finite SWNTs belonging to a given family k exhibit strikingly similar oscillating patterns (when plotted in terms of *even* NT sections) with diminishing amplitudes from the armchair, to chiral, and to the zigzag SWNTs. However, in terms of the NT length, the gap maximum repeat at different periodicities for different SWNTs. We find that ASWNT at selected lengths behave as semiconductors, in contrast to the metallic behavior of infinite ASWNTs. On the other hand, infinite ZSWNTs which can be either metallic or semiconducting behave as molecular-scale conductors. These results are expected to have profound implications in the utilization of finite-length CNTs as molecular-scale devices.

PoS Su30 15.30-18.30

Formation Mechanism and Packing of Nanotube Peapods

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We investigate the absorption process and the packing geometry of fullerenes in nanotubes and peapods using molecular dynamics simulations and structure optimization techniques. To understand the way a fullerene enters a nanotube to form a ``nano-peapod'', we investigate the absorption dynamics of a C_{60} molecule in a (10,10) nanotube either through the open end or a large opening in the tube Wall. The underlying Linear Combination of Atomic Orbitals total energy functional is based on *ab initio* calculations. Our results for the C_{60}@(10,10) system suggest that the most efficient absorption occurs through defects in the tube Wall, within a narrow launch velocity window that corresponds to the experimentally observed optimum temperature range for peapod formation. In an open system containing fullerenes and peapods, the energy gain associated with fullerene entry into the tube exposes the encapsulated fullerenes to an internal pressure which can amount to a fraction of one GPa. This pressure reduces the inter-fullerene separations, and could be used to compress other substances within the tubes.

PoS Su31 15.30-18.30

TEM and SFM Investigation of Single Walled Carbon Nanotubes Grown by CVD Between Microprinted Catalyst Islands

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Single-walled carbon nanotubes were grown between catalyst islands by chemical vapor deposition of methane and hydrogen. The deposition of the catalyst was performed using microcontact printing. This allows to produce a large number of samples with different patterns in much shorter time compared to electron beam lithography normally used to define catalyst positions. To charcterize the grown tubes, e.g. with respect to their exact diameter or the number of walls, it is crucial to examine them by transmission electron microscopy (TEM). Therefore the catalyst pattern was microprinted on ultrathin (20nm) silicon nitride substrates that are transparent for electrons and suitable for scanning force microscopy (SFM) as well. Thus it was possible to routinely study the obtained as-grown nanotube arrangement by TEM and SFM. In our investigation high quality individual single-walled carbon nanotubes with a broad diameter distribution were found, together with various types of crossings and junctions.

PoS Su32 15.30-18.30

Non-Contact Scanning Force Microscopy Induced CVD: First Attempts Towards Contacting Nanotubes on an Insulating Substrate

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Using a Scanning Force Microscope (SFM) a new single-step additive process is investigated for electrically contacting carbon nanotubes (CN) on a non-conducting surface. To this effect, vapors of a organometallic precursor are adsorbed to the surface of a substrate with pre-patterned conducting regions, e.g. wiring patterns to which pre-deposited nanotubes on the surface shall be connected. In non-contact imaging mode the SFM tip can be positioned on a conducting region from which a contact is to be made to a CN. A bias voltage is applied between the conducting cantilever/tip and the conducting regions of the sample, resulting in the formation of metal containing deposits at the tip location. Starting from the conducting region the tip is moved across the non-conducting region where adsorbed organometallic molecules are decomposed to form metallic features while the tip-sample current is monitored. In this way a conducting bridge from the patterned electrodes to the CN could be formed. This procedure can be performed at room temperature in air with a reservoir of organometallic material close-by. While a similar effect has been previously obtained using a scanning tunneling microscope on conducting substrates, the exact nature of the SFM-based process is still being investigated.

PoS Su33 15.30-18.30

Direct Nano - Bridging of Carbon Nanotube Using Growth Barrier for Nanoelectronics: A Possible Mechanism of Selective Lateral Growth and Observation of Field Effect

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We have fabricated carbon nanotube field-effect transistor of a direct nano-bridged between micro-sized Ni electrodes using conventional photolithography technique. Especially, in this work we introduced a growth barrier of Nb metal or insulating layer on the top of the catalytic metal to prevent the growth of CNW from vertical direction to the substrate. As a result, CNTs were selectively grown between lateral sides of the Ni electrodes with pre-defined Nb external terminals. We have demonstrated the ability of this three thermal structure with back gate to provide field effect of conductance modulation ability of 3-4 orders of magnitude as a function of gate voltage at room temperature. This is the first report on the field effect of the directly bridged CNT-FET with catalytic metal electrodes. We ensure that this will greatly simplify fabrication process so that a large number of nano-electronic devices can be formed by combining cost-effective CVD method at low temperature with a commercially available 1.2 micrometer MOS process.

PoS Su34 15.30-18.30

Temperature Dependence of Field Effect Function of a Direct Bridged CNT Between Ferromagnetic Electrodes: Ni as Both Catalyst and Contact Electrode

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The temperature dependences of the field effect of a direct nano-bridged carbon nanotube (CNT) between micro-sized Ni electrodes were studied in the range of 100-300 K under back-gate biasing. CNTs were selectively grown between the lateral sides of the Ni electrodes with pre-defined Nb external terminals. The temperature dependence of two-terminal resistance showed a thermal activation at high temperatures in all samples measured. At the room temperature linear resistance of Ni-CNT-Ni structure showing field effect function was about 5 megaohm. The normalized resistance R(T)/ R(300K) increases three or five orders of magnitude from 5megaohm to gigaohm range as the temperature is lowered from 300 to 80 K, showing nearly insulating transition. The differential conductance versus bias voltage spectrum showed energy gap (E) of ~1.4 eV at 100 K and this value corresponds to the outer diameter d of about 1.6 nm from the relation of energy gap(E) ~ 1/d. Considering E_g =1.8 eV for a single Wall nanotube with diameter of 1.3 nm, the estimated value is reasonable. We also observed an interesting temperature and time dependence of device characteristics and will discuss their implication in terms of intrinsic and extrinsic properties of the devices.

PoS Su35 15.30-18.30

Computational Studies of Catalysed Nanotube Growth

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Although metal catalysts are often used in the production of single-walled carbon nanotubes (SWNTs), the catalytic growth mechanism is not fully understood. Increased knowledge of the role of the catalyst in nanotube nucleation and production is not merely of fundamental interest, but will also assist in the quest to manufacture separate, defectless SWNTs that have a desired chirality. In spite of this there has been a relatively limited number of computational studies of catalysed nanotube growth. This is due, in part, to the long time required for growth and the difficulty of modelling transition metal catalysts accurately. In this work we discuss ab initio and semi-empirical methods to study iron-catalysed SWNT production. Ab initio calculations, which are computationally expensive, yield accurate structural and geometric information, and semi-empirical direct dynamics simulations provide insight into the catalytic growth mechanism.

PoS Su36 15.30-18.30

Formation Mechanism of Single-Wall Carbon Nanotubes and Single-Wall Carbon Nanohorns

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Formation mechanism of SWNTs is controlled by metal particles with nanometer-sized diameters, probably 1 to 2 nm, and the metals effective to grow SWNTs are good graphitization catalysts, have low solubility in graphite, and the crystallographic orientation on graphite is stable. On the other hand, single-Wall carbon nanohorns are formed only from graphite. single-Wall carbon nanohorns are formed in an atmosphere where density and temperature of carbon are extremely high, which is realized in the laser plume.

PoS Su37 15.30-18.30

Coalescence of Fullerenes in Single-Walled Carbon Nanotubes

Kaori Hirahara [1], Shunji Bandow[2], Masako Yudasaka[1], Kazutomo Suenaga[1] and Sumio Iijima[12]

1 'Nanotubulites', Japan Science and Technology Corporation
2 Department of Materials Science and Engineering, Meijo University

To understand the growth mechanism of inside tube, we performed the heat-treatments of peapods at various temperatures below 1200°C and examined by a transmission electron microscope. The structural changes of the inside C_{60} can be seen when the heat-treatment were done at > ~800°C.

For the sample heated at 800°C (HT800), we observed a smaller intermolecular distance for a pair of fullerene molecules, which are part of a long fullerene chain, than that of original peapods. Therefore it is natural to consider the existence of chemical bond between adjacent fullerenes. For HT900, peanut-like shaped $C_{120}^{\pm}{}_{x}$ molecules are conspicuously observed, which are made by coalescence at a contact region between two fullerene molecules. Further heating at 1200°C, a neck growth of the peanut results in an elliptical shape. For HT950, such cages or short nanotubes can be seen more frequently. For HT1000, the probability of fullerene coalescence is increased and therefore many longer secondary tubes are generated. At around this temperature, the fullerenes are fused together and simultaneously the re-organization of C atoms occurs to adjust the diameter of secondary tubes to the host nanotube. For HT1200, all fullerenes are converted to naotubes.

Upon the above observations, we propose the model for metastable structures observable during the transformation from a fullerene chain to an inside tube.

Abstracts Monday

Mo1 A 8.30-9.15

Carbon Nanotube-Based Hybrid Materials

David E. Luzzi

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Nanoscale hybrid materials are composed of nanotubes in which the interior core is filled with atoms, molecules or materials. There has been a growing interest in nanotube-based hybrid materials due to the modification and control of properties and novel functionalities inherently possible in this class of materials. Indeed, when the outstanding properties of the nanotube are combined with those of interior molecules, it is conceivable that tri- or quad-functional smart materials can be produced. Recently, we have shown, using C_{60}, that these materials can be produced using synthesis routes amenable to bulk production. The synthesis involves transport of C_{60} molecules in the gas phase to partially-oxidized SWNTs where they enter through open ends and side-Wall defects, forming linear chains. The process is efficient and yields high concentrations of SWNTs filled over long lengths. Another example is the endohedral molecule $La_2@C_{80}$. This molecule is interesting due to the large electron transfer that is predicted by first principle calculations. Interestingly, within the SWNT, the La-La atom separation is greater than 0.5 nm, significantly larger than the 0.36 nm predicted from ab-initio calculations of the isolated endohedral. In addition, the dynamics of rotation of the endohedral molecules is modified within the SWNT versus in solution suggesting a strong interaction with the surrounding SWNT. Results on the filling of SWNTs with C_{60} and other molecules and materials will be presented along with the results of electrical and thermal property measurments of the resultant hybrid materials. Anneals of C_{60}0-filled SWNTs at high temperatures produces molecular coalescence of the C_{60} chains into hemispherically-capped capsules and long tubes. Some of the produced structures are present in a metastable structural form. This work demonstrates that SWNTs can be used as nanoscopic reaction chambers for the production of new molecules. The SWNT plays a dual role of catalyzing the reaction by controlling the orientation and proximity of the reactants and as a steric template that limits the attainable conformations of the reaction product.

Mo1 B 9.15-10.00

Carbon Nanomaterials in Heterogeneous Catalysis

R. Schlögl, G. Mestl, E. Sanchez, N. Maximova

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Nanostructured carbons such as fullerenes, fullerene black, nanotubes and other objects exhibit an unusual ratio between basal and prismatic faces at their surfaces. In addition, the localisation of olefinic bonds creates unique reactivity as ligand and anchoring site for metal particles to be supported on carbon. The differing chemical functions of basal and prismatic carbon faces will be illustrated. Fullerenoid structures are too reactive to be used as stable catalysts. Multi-walled nanotubes, however, show unique and promising properties as catalysts for selective hydrogenation and oxidation reactions. Facile synthesis methods will be discussed allowing to utilize these structures in technical quantitites.

Mo2 A 10.30-11.15

Controlling the Electronic Properties of Carbon Nanotube Bundles

Philip G. Collins, Richard Martel, Phaedon Avouris

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Ideally, a carbon nanotube is a unique, low-dimensional conductor which can have either metallic or semiconducting properties. In practice, however, these hollow cylinders have a strong tendency to agglomerate as they form, resulting in either large, multi-walled nanotubes (MWNTs) with many concentric carbon shells or else bundles, or "ropes," of aligned single-walled nanotubes (SWNTs). Both aggregates are complex composite conductors incorporating many weakly-coupled nanotubes, each having a different electronic structure. We will demonstrate a simple and reliable method for selectively removing single carbon shells from MWNTs and SWNT ropes to tailor the properties of these bundled nanotubes. The technique allows us, for the first time, to step through and individually characterize the different shells of a MWNT. By choosing from among the different shells, we can convert a MWNT into either a metallic or a semiconducting conductor, as well as quantitatively address the issue of inter-shell transport. With SWNT ropes, similar selectivity allows us to generate entire arrays of high performance, nanoscale field-effect transistors (FETs) based solely on the fraction of semiconducting SWNTs. These procedures sidestep the need for selective nanotube synthesis and allow unprecedented flexibility in the study of both nanotube physics and nanoscale electronic devices.

Mo2 B 11.15-12.00

When Are Carbon Nanotubes Ballistic Conductors?

Walt A. de Heer

School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA

Frank, de Heer et al (Science 280,1744 (1998) found that freely suspended multiwalled carbon nanotubes (MWNTs) are 1-D conductors; the current flows on the outer layer, while large current densities are sustained. Quantized conductance was also found. These findings imply that carbon nanotubes could be ballistic conductors at room temperature. However there are difficulties that need clarification. One is that the conductance is only half what is expected from the theory of single Wall nanotubes. Experiments performed on substrate supported and lithographically contacted nanotubes do not (yet) exhibit quantized conductance. Moreover electrical transport in carbon nanotubes is still quite confusing. Our experiments show that the conductance of clean, well-contacted nanotubes is quantized and independent of intercontact distance. Contamination, defects, non-ideal contacts and substrate interactions may explain the discrepancies between our experiments and others.

Mo3 A 13.30-14.15

Recent Transport and STM Results on Carbon Nanotubes

Cees Dekker

Delft University of Technology, Lorentzweg 1, Delft, 2628 CJ, The Netherlands

This talk will review recent work on electrical transport through single-Wall carbon nanotubes as carried out in our group at Delft. With STM experiments we have mapped out the two-dimensional molecular orbitals of tubes. A long wavelength amplitude modulation is observed which allows to extract the Fermi velocity and the linear dispersion relation. Recent transport experiments include work on a room-temperature single-electron transistor that was made from a single nanotubes by inducing two barriers by local AFM manipulation.

Mo3 B 14.15-15.00

Theoretical Study of the Quantum Conductance of Nanotube Structures: Defects, Junctions, and Peapods

Steven G. Louie

Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

In this talk, I discuss the quantum conductance of several carbon nanotube structures, calculated using the Landauer-Büttiker formalism. Systems examined include tubes with local defects, crossed nanotube junctions, and nano-peapods. Ab initio calculations show that local defects such as impurities and pentagon-heptagon pairs often produce sharp, quantized reductions in conductance due to resonant backscattering by defect states. The structural deformation and transport properties of crossed carbon nanotube junctions on a substrate are investigated as a function of applied force on the junction. We find that the intertube junction conductance can be sizable and is sensitive to the external applied force. We have also carried out calculations on the electronic structure and conductance of nano-peapods. Results for isolated fullerenes (with or without endohedral atoms) and those for a one-dimensional chain of fullerenes in single-walled carbon nanotubes are presented. The influence of fullerene molecular states on tube conductance is described. Finally, we present some calculated results on the I-V characteristics of on-tube metal-semiconductor junctions.

PoS Mo1 15.30-18.30

Multiwalled Carbon Nanotubes as Nanoscale Electronic Devices

M. Ahlskog, R. Tarkiainen, L. Roschier, and P. Hakonen

Low Temperature Laboratory, Helsinki University of Technology, Espoo, Finland

Carbon nanotubes may form the building blocks of future nanoscale electronic devices. We have measured the electronic characteristics of single electron transistors (SET) fabricated from multiwalled carbon nanotubes (MWNT) in various configurations. Moreover, we have used MWNTs synthesized both by the arc-discharge (AD) and chemical vapour deposition (CVD) methods. Both the mechanical and electronic properties of these tubes are very different. Generally CVD tubes have a clearly higher density of defects. In devices fabricated from AD tubes we observe clear Coulomb blockade oscillations at low temperatures. In a SET where the central island is formed by a MWNT, a second MWNT crossing the former can be utilized to gate the source-drain current. In another device where the MWNT is suspended above the substrate between the electrodes, we measure an extremely high charge sensitivity of $6x10^{-6}$ e/sqrt(Hz) at 45 Hz, comparable to the best of the conventional SETs. In CVD tubes we measure a clearly higher resistance and irregular Coulomb blockade oscillations.

PoS Mo2 15.30-18.30

A Study on the Electrical Transport in and Between Single-Wall Carbon Nanotubes

J. Appenzeller [1], H. Stahl [2], B. Lengeler[2], R. Martel [1], Ph. Avouris [1]

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[2] *Physikalisches Institut, RWTH Aachen, 52056 Aachen, Germany*

By intentionally damaging ropes of single-Wall carbon nanotubes through a controlled Ar-sputter treatment, we are able to characterize the electrical coupling between metallic nanotubes and to study coherent transport within metallic tubes with respect to the dominant phase breaking scattering mechanisms. Introducing sputter-damage to nanotubes in a rope, while preserving their structural integrity, enables to influence the current path through a rope as a function of temperature - meaning that at low enough temperatures current switches from one metallic tube to another one. Studying and modeling this process in detail is a possibility to thoroughly characterize the intertube barriers as well as the coupling mechanism between tubes in a rope. Our observations clearly proof that direct tunneling through a 250meV barrier posed by the semiconducting tubes in the rope is the dominant coupling mechanism. In addition, our data allow to characterize phase coherent transport in metallic nanotubes and to identify electron-electron scattering as well as Thouless scattering as the two relevant scattering processes dominating the coherent transport between 4K and room-temperature.

PoS Mo3 15.30-18.30

Electronic Transport in Multi - Walled Carbon Nanotubes

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[2] *Institut de Génie Atomique, EPFL, CH-1015 Lausanne, Switzerland*

We have studied the differential conductance of single multi-walled carbon nanotubes (MWNT's) as a function of bias and gate voltage. Clear traces of coulomb blockade could be observed for MWNT's connected to Au electrodes, even when the average two-terminal conductance was high (~$2e^2/h$ at 280 mK). At such intermediate Au - MWNT transparancies, i.e. low enough to see the remainders of coulomb blockade and high enough to reach conductances of $2e^2/h$, one can expect higher-order tunnelling processes to play an important role in the electron transport. An example of such is the Kondo effect which was observed for the first time in single Wall tubes by Nygard *et al* [1]. We obtained very similar results on a MWNT and studied the Kondo resonance as function of temperature and magnetic field. Preliminary measurements of MWNT`s contacted to superconducting electrodes show a considerable resistance drop below the T_C of the contacts. Upon applying a small magnetic field, the sample behaves similar to measurements performed with normal gold contacts. [1] Nygard. J *et al*. Nature **408**, 342 (2000).

PoS Mo4 15.30-18.30

Electronic Transport and Structure in Carbon Nanotube Junctions

Hyoung Joon Choi[1], Jisoon Ihm[2], Young-Gui Yoon[1,3], Steven G. Louie[1,3], and Marvin L. Cohen[1,3]

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With an intramolecular junction of a metallic and a semiconducting carbon nanotube, we study the electronic current and structure along the junction at finite bias voltage using a self-consistent tight-binding method. The atomic arrangement and charge redistribution along the junction at finite current density are taken into account in our calculation by nearest-neighbor hopping of π-electrons and by a self-consistent Hartree-type electrostatic interaction among the electrons. Our result shows zero current at smaller bias voltage than the bandgap of the semiconducting tube, and superlinear increase of current at larger bias voltage. The self-consistent charge density shows maximal fluctuation of 3 percents in the 1 nm long region at the junction, and smaller Friedel oscillation in the metallic part. The screened electrostatic potential, at finite bias voltage, is almost constant in the metallic part and drops linearly in the semiconducting part.

PoS Mo5 15.30-18.30

Electronic Transport in Ultra-Clean Single-Walled Carbon Nanotubes

M. S. Fuhrer[1], A. Bachtold[2], M. Forero[2], A. Zettl[2], Paul L. McEuen[2]

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[2] *Dept. of Physics, University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley CA, 94720 USA*

Devices consisting of individual CVD-grown carbon nanotubes up to ten microns long contacted by gold electrodes have been fabricated. By using electrostatic force microscopy to image the local potential in current-carrying devices, the mean free path in both semiconducting and metallic nanotubes has been measured. Individual scattering sites in semiconducting nanotubes can also be studied by monitoring the nanotube conductance while using the AFM tip as a local gate. CVD-grown nanotubes are exceptionally free of disorder: room temperature mean free paths of up to 700nm are possible in CVD-grown semiconducting nanotubes. Low temperature transport measurements indicate that the mean free path in semiconducting nanotubes may be as long as 6 microns. Results on these semiconductor quantum dots will also be discussed. A new electrically-programmable memory device based on a single semiconducting nanotube will also be presented.

PoS Mo6 15.30-18.30

Multiwalled Carbon Nanotube: Luttinger Liquid or Not?

R. Tarkiainen[1], M. Ahlskog[1], J. Penttil[1], L. Roschier[1], **P. Hakonen**[1], M. Paalanen[1], and E. Sonin[1,2]

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At low voltages, the tunneling conductance obeys non-Ohmic power law, which is predicted both by the Luttinger liquid and the environment-quantum-fluctuation theories. However, at higher voltages we observe a crossover to Ohm's law with a Coulomb-blockade offset, which agrees with the environment-quantum-fluctuation theory, but cannot be explained by the Luttinger-liquid theory. From the high-voltage tunneling conductance we determine the transmission line parameters of the nanotubes. For the kinetic inductance we obtain l_{kin} = 0.5 mH/m, which indicates that the average number of conducting layers in our nanotubes is 8 (out of about 20) at frequencies of f = 0.5 - 10 THz.

PoS Mo7 15.30-18.30

Transport of Annealed MWCNT and its Application to Transistor Device

Jaeuk Chu[1], Kwangseok Jeong[1,2], Eunju Bae[1,2] and Wonbong Choi[1,2], Minho Yang[3], Seahn Song[3] Hyoung Joon Choi[1], Jisoon Ihm[2], Young-Gui Yoon[1,3]

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[2] *The National Program for Tera-level Nanodevices*
[3] *Analytical Engineering Center, Samsung Advanced Institute of Technology, Suwon, Korea*

Highly ordered nano hole array on Anodic Aluminum Oxide(AAO) was fabricated by two step anodization method and MWCNTs were grown selectively in AAO template with thermal CVD at the temperature range of 600~700C. The interface between MWCNT and metal electrode was modified by long time annealing. High temperature annealing in N_2 flowing change the tube-metal system into the tube-oxide-metal interface, which is observed by TEM. I-V characteristics of annealed MWCNT shows non-linearity at room temperature and its resistivity r is about 1.3×10^{-6}W cm. The modified interfacial structure has an influence on I-V characteristic as the coulomb blockade. It was shown that the electric current was gate-bias dependent. In this talk, we will discuss various patterned gate structures of CNT/Al_2O_3/Al/ system using conventional and e-beam lithography and their electrical properties related to structural changes.

PoS Mo8 15.30-18.30

Conductance of Multi-Wall Carbon Nanotubes

Anders Hansson, Magnus Paulsson, and Sven Stafström

Linköping University

The aim of this theoretical work is to find methods to control the current through multi-Wall carbon nanotubes (MWNTs). In our model system the tight-binding approximation is used to describe a finite MWNT ((10,10)@(5,5)) connected to two semi-infinite metallic leads. The current-voltage characteristics is calculated from the multi-channel Landauer formula. Changes in the on-site energy, the interaction between layers of the MWNT and interaction with the leads are investigated to determine how they affect the conductance. In the experimental situation this corresponds to applying a gate voltage either to the underlying substrate or to a microscopy-tip. The interaction between the layers may also be increased by mechanically deforming the MWNT with the tip. In the case of weak interaction between the leads and MWNT the calculations show that the conductance mainly depends on the wavefunction amplitude on the sites connecting the MWNT to the leads. The elastic scattering induced by defects thus does not necessarily decrease the current through the MWNT. A device in which the leads are contacted to different coaxial layers of the MWNT (telescopic junction) is also investigated and the sensitivity to defects studied.

PoS Mo9 15.30-18.30

Anderson Localization in Metallic Carbon Nanotubes

M. Hjort and S. Stafström

Linköping University, Sweden

Experimentally, the electron localization length is found to be very large in metallic NT's, regardless of tube chirality. A long localization length is important for the ballistic transport properties of the NT's, and depend crucially on the amount of disorder present in the tube. So far has only disorder induced localization, so called Anderson localization, been studied quantitatively for armchair NT's. We study for the first time also the much more complex chiral NT's, using the transfer matrix method. The electron localization due to diagonal disorder is shown to be independent on chirality and the localization length is in total agreement with the values reported for armchair NT's. Especially, we consider functionalization of the NT's as a diagonal disorder for which the conductance will decrease exponentially with the number of functionalized atoms. This effect may be used in applications where NT's act as sensors. Functionalization in this case also includes atom substitution and gas adsorption, and we have particularly studied the effect of oxygen adsorption.

PoS Mo10 15.30-18.30

Barrier Formation in Electrical Contacts Between Metal and Multi-Wall Carbon Nanotube

A. Kanda [1,2], K. Tsukagoshi[3], Y. Ootuka[1,2], and Y. Aoyagi[3]

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[2] *CREST, Japan Science and Technology Corporation, Japan*
[3] *The Institute of Physical and Chemical Research (RIKEN), Japan*

For the application of carbon nanotubes to molecular electronic devices, it is very important to control the contact resistance between metal and a nanotube. In order to get information on the origin of contact resistance, we have studied material dependence of the electrical transport in metal/MWNT/metal structure in metal-on-tube configuration. When the metal was Ti, the room temperature resistance ranged from 28 k Ohm to 45 M Ohm, and all of the samples cooled to 30mK showed the Coulomb blockade (CB) effect. The total junction capacitance estimated from the CB was proportional to the length of MWNT segments overlapped by Ti electrodes, showing that the tunnel barrier was located in the Ti-MWNT contact. When the metal is Au with the sticking layer of Pt, on the other hand, resistance distribution shifted to a much lower value in comparison with Ti, though the fabrication process was the same. This shows that the contact resistance comes from the mismatch between MWNT and the metal. One possible origin of high contact resistance is oxidation of the metal surface touching the MWNT.

PoS Mo11 15.30-18.30

Effects of a Perpendicular Magnetic Field on the Nanotube Conductivity

Alex Kleiner and Sebastian Eggert

Theoretical Physics, Chalmers, Goteborg, Sweden

We study theoretically the conductivity of a metallic nanotube under a perpendicular magnetic field. The density of states and the backscattering probability vary with the field, resulting in fluctuations of the conductivity as a function of the magnetic field.

PoS Mo12 15.30-18.30

Band Gap Modification by Circumferentially Perturbing Potentials in Carbon Nanotubes

Yong-Hyun Kim and K. J. Chang

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When single-Wall carbon nanotubes are placed in potential environments such as metal electrodes, gate potentials, flattening deformations, and transverse electric fields, their electronic and transport properties are significantly modified. In very recent theoretical calculations [1], flattening deformations have shown to induce the band gap modification such as opening and closure, and locally deformed carbon nanotubes have been demonstrated to behave as quantum dots or wires [2]. However, the effects of metal electrodes and transverse gate fields on the transport properties have not been studied yet. In this work, we analyze the periodicity of external potentials induced by electrodes and gate fields along the circumference direction in a perturbative way. We find that selection rules exit in the subband mixings caused by perturbations. We also perform first-principles pseudopotential and tight-binding calculations to calculate the electronic structure of single-Wall carbon nanotubes under transverse electric fields. We find that semiconducting nanotubes undergo a semiconductor-metal transition as the field strength increases, while transverse electric fields open the band gap of metallic nanotubes. We demonstrate the band gap engineering by external perturbations and the applications of nanotubes for nano-scale devices. [1] C.-J. Park, Y.-H. Kim, and K. J. Chang, Phys. Rev. B **60**, 10656 (1999). [2] H.-S. Sim, C.-J. Park, and K. J. Chang, Phys. Rev. B **63**, 73402 (2001).

PoS Mo13 15.30-18.30

Electrical Transport Properties in Multi-Wall Carbon Nanotube p-p Hetero-Junction

J.-O. Lee, H. Oh, J. -R. Kim, K.C. Kang, and J.J. Kim, J. Kim , J. W. Park, K.H.Yoo

Chonbuk National University and Korea Research Institute of standards and Sciences.

We have studied the electronic transport properties of hetero-structure junction made of two different multi-Wall carbon-nanotubes. The independent measurements on each nanotube revealed that the one show p-type semi-conducting behavior with a gap size of about 300 mV, the other also was p-type semi-conductor with a gap size of about 80 mV. The measured current-voltage characteristics across the hetero-junction show reproducible rectifying diode behavior with highly non-linear transport properties. The forward bias current across the junction increased strongly with increasing the gate bias voltage positively indicating n-type gate response. This diode behavior and n-type gate modulation could be explained by the bending effect of valence band in the hetero-junction

PoS Mo14 15.30-18.30

Single Wall Nanotube Field-Effect Transistors and Logic Circuits

R. Martel, V. Derycke, C. Lavoie, P. Wong, and Ph. Avouris

IBM T. J. Watson Research Center

One of the most interesting applications of carbon nanotube involves their use as active channels of field-effect transistors (FETs) [1]. The transconductance of these early devices was small (10^{-9} A/V), limited by the resistance of the contacts. We will present new results on nanotube FETs with optimized performance. We found that the "on" and "off" currents as well as the transconductance of the devices depend strongly on the properties of the junction between the source-drain metal and the nanotubes. By optimizing this geometry using carbide contacts, we have achieved several order of magnitude higher transconductances and the carrier mobilities now exceed 100 cm^2/Vs. These devices show bipolar transport (p- and n-type) resulting from the weak Fermi-level pinning of the contacts. The detail of the transport mechanism in these devices will be presented. Their characteristics will also be benchmarked with the silicon MOSFET and shown to be comparable. Finally, we demonstrated the fabrication of various logic circuits based on nanotubes using complementary p- and n-type nanotube FETs. [1] S. J. Tans et al. Nature 393, 49 (1998); R. Martel et al. Appl. Phys. Lett., 73, 2447 (1998)

PoS Mo15 15.30-18.30

Electronic Transport Behaviour in Carbon Nanotube Ropes

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In this presentation we emphasize interesting behaviour observed for the electronic transport properties of two single-walled carbon nanotube (SWCN) rope samples. For the first sample, the Coulomb blockade regime has been explored. The Coulomb blockade peaks observed display interesting three-way splitting, the cause of which can be related to resonant tunnelling through discrete energy levels of a finite length metallic SWCN within the rope. We also consider the possible role that interactions between `quantum dot' regions within the rope can play in causing such peak splitting. For the second sample, we have explored magnetoresistance behaviour. For a magnetic field applied perpendicular to the rope axis we observe monotonic negative magneto-resistance due to two-dimensional weak localisation within the rope. By contrast, for a magnetic field applied parallel to the rope axis we observe complicated oscillatory behaviour due to the Altshuler-Aronov-Spivak effect. One particular oscillatory mode can be identified which corresponds to closed cylindrical paths around the outer diameter of the SWCN rope. However, overall, due to the composite filamentary nature of the rope and the multitude of closed electron trajectories available, the complicated oscillatory behaviour can be classified as universal conductance fluctuations.

PoS Mo16 15.30-18.30

Wave-Vector Conservation and Electric Transport Through Crossed Carbon Nanotube

Takeshi Nakanishi[1] and Tsuneya Ando[2]

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Carbon nanotubes (CNs) are new kinds of quantum wires with particular transport properties. A junction of two crossed nanotubes is likely to be a fundamental element to form multiterminal molecular devices using CNs. The purpose of this paper is to study electric transport through crossed single-Wall CNs and to demonstrate the importance of wave-vector as well as energy conservation. An effective-mass scheme has been used successfully in the study of wide varieties of electronic properties of CNs including transport properties. In this paper the effective-mass scheme is extended to junctions of crossed CNs and an effective Hamiltonian describing their coupling is derived. For a realistic model, it turns out that effective coupling between two tubes is reduced considerably due to interferences of couplings between different atoms except when hexagons on two CNs stack in a commensurate way. As a result dominant components of the effective couplings take sharp and high peaks as a function of the angle between the tubes. The conductance between two metallic armchair CNs is calculated and shown to have a sharp maximum at the peaks of the dominant components and be negligibly small except for these peaks.

PoS Mo17 15.30-18.30

One-Dimensional Localization in Single-Wall Carbon Nanotubes

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NEC Laboratories, ICORP-JST, Meijo Univ.

Single-Wall carbon nanotubes (SWNTs) have been intensively studied because of their peculiar electronic properties. SWNTs are either one-dimensional metals or semiconductors, depending on their diameter and chirality. Thus transport measurements on each individual SWNTs are required to reveal their inherent properties. We report one-dimensional localization in an semiconducting SWNT. As-grown SWNTs were directly dispersed on a saphire substrate in order to reduce the formation of bundles and the creation of damages during the purification processes. Attachment of Ti electrodes to a SWNT followed by heat treatment was carried out to make ohmic contacts. The temperature dependence of the two-terminal resistance showed $\exp[(T_0/T)^{(1/2)}]$ dependence, where $T_0=5.4\text{x}10^4$ K. This temperature dependence implies that one-dimensional variable range hopping dominates this semiconducting SWNT.

PoS Mo18 15.30-18.30

Kondo Effect in Carbon Nanotube Quantum Dots

Jesper Nygård[1], David H. Cobden[2] und Poul Erik Lindelof[1]

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For single-Wall nanotubes, the electron transport at low temperature is often dominated by Coulomb blockade effects due to tunnel barriers formed between the nanotubes and the attached metallic electrodes. We have obtained low-resistance contacts to single-Wall nanotubes, enhancing the higher-order cotunneling processes, and have observed the Kondo effect in such a "quantum dot" [1]. Here, a resonance for transmission exists at low temperature due to the formation of a many-body state involving an unpaired spin on the tube and the conduction electrons in the gold leads. The one-dimensionality of nanotubes makes the effect particularly pronounced, with Kondo temperatures up to 2 K and for large electron number *N*. The effect exist only for odd *N*, reflecting even-odd alternations due to spindegeneracy. However, at finite magnetic field an effect induced by a singlet-triplet degeneracy is observed for even *N*. [1] Nygård, J., Cobden, D.H., and Lindelof, P.E., Nature **408**, 342 (2000).

PoS Mo19 15.30-18.30

Electrical Transport in Nanotubes With Realistic Contacts: An Ab-Initio Study

J. J. Palacios, A. J. Perez-Jimenez, E. Louis, and J. A. Verges

Universidad de Alicante and ICMM

We present an ab-initio study of the electrical transport properties of fullerenes and short nanotubes contacted to metallic electrodes. The part of the electrodes that is close to the contact with the molecules, is described at the atomic level and treated at the same level of approximation as the nanotubes. Far away from the contacts, where the details are unimportant, the electrodes are described by Bethe lattices. This allows us to estimate the contribution of the semiinfinite parts of the system in a simple manner. We show that a good description of the charge transfer at the contact region is essential to obtain the correct band structure and to understand the transport properties of these molecules in actual experiments.

PoS Mo20 15.30-18.30

Multiwalled-Carbon Nanotubes as Non-Ballistic Conductors

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Intrinsic geometry of multi-walled carbon nanotubes allows to differentiate between long-ballistic, anomalous and diffusive-like conductors. Specific length scaling of the electronic conductance and temperature dependence of inelastic scattering times and conductivities in the weak electron-electron regime are predicted.

PoS Mo21 15.30-18.30

Influence of Length on the Electrical Transport into Metallic, Semiconducting, and M-S Junction Carbon Nanotubes

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One of the most important findings of carbon nanotubes (CNTs) research is that the current in semiconducting tubes can be switched by an external electric field which allows semiconducting tubes to be used as the channel of field-effect transistors (FETs). So far, the NT segments used in the FET experiments have been relatively long, in the order of several hundred nm to a micron. However, the process of device miniaturization aims primarily at reducing the channel length. The question then arises if short nanotube devices can preserve the operational characteristics of long devices. We have investigated theoretically the influence of the length on the electrical properties of two general types of CNT named metallic (M) and semiconducting (S) tubes, and a third type made of both M and S tubes called a M-S junction. We compare the variation of electronic and electric properties with the length of NTs in a 0-20 nm range. The electronic structure calculations on M and S CNTs clearly show a transition from 0-D (molecular) to 1-D (wire) between 2.5 and 5.0 nm. The changes are more subtle for the M-S junction due to the electronic structure mismatch between the M and S segments at the interface. The variation of electrical transport properties are discussed in terms of the presence of discrete molecular orbitals in short CNTs, the contribution of electron tunneling, and to the presence of metal-induced-gap states (MIGS).

PoS Mo22 15.30-18.30

Resonant Tunneling in Carbon Nanotubes in Presence of Two Tunneling Junctions

M. Thorwart, M. Grifoni, H.W. Ch. Postma, and C. Dekker

Delft University of Technology

We investigate theoretically resonant tunneling in nanotubes containing two sharp bends. Because the bends act as tunneling junctions, the system constitutes a one-dimensional quantum dot attached to one-dimensional leads. The linear as well as the nonlinear transport are investigated within a master equation approach as well as by means of precise *ab initio* real-time path-integral simulations. By treating the strong Coulomb interaction among the quasi-one-dimensional electrons within the framework of Luttinger liquids, a characteristic power-law behavior for the differential conductance is extracted. Our results are applied to explain recent experimental findings for transport in metallic nanotubes containing two sharp bends. These local deformations, acting as tunnel junctions, have been designed with the tip of an atomic force microscope.

PoS Mo23 15.30-18.30

Real Space Imaging of Interfering Bloch Waves on Carbon Nanotubes at Room Temperature

A. Hassanien[1], P. Umek[2], A. Mrzel[2], M.Tokumoto[1] and D. Mihailovic[2]

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We report on the structure and the electronic properties of single wall carbon nanotubes tips with atomically spatial resolution. Topographic STM images reveal variety of geometrical structure of closed tips; these include round, conical, as well as tips with a messy shape. Standing wave pattern of the charge density is observed at the tube cap which depends strongly on the bias voltage. The pattern is formed due to constructive interference between the electronic states and its reflection on the nanotube tips. Atomically resolved images show asymmetry in the charge density that decays out within 6 nm away from the cap. These distinctive tip states do not exist elsewhere on the tube and are related to the presence of topological defects at tube ends.

PoS Mo24 15.30-18.30

New Opportunities Lead to New Roles for Science and Business

Silke Burkart, Silvester Schmidt

TIMElabs Research Center @ Diebold, Eschborn, Germany

Nanotechnology is far more than a fascinating scientific discipline or an emerging market, even more than the sum of both. Working in an innovation-driven and globalized environment, players from science and business face new challenges: Nanotechnology is strongly supported by politics, research is done in multinational networks and companies are spending large amounts on basic research. The interest in research is changing from purely scientific to business-oriented, so that some multi-national companies are spending a large amount of their annual R&D budget on basic nanotechnology research. Some of the best known companies with focus on nanotechnology have as yet no available products but do a lot of marketing for their research projects. Companies and scientific institutes have developed different ways to solve the problem of shortening the time-to-market for research-intensive products through new forms of cooperation. These range from research cooperations to complex virtual companies. Out of these new ways to cooperate, new business models can be developed. The change in the roles of science and business will be so profound that corporate organizational structures will be affected as well as the tasks and required capabilities of management and staff.

Mo AD 20.00-21.00

Perspectives on the Role of Carbon Nanotube Research in the Worldwide Nanotechnolgy Initiative

Mildred Dresselhaus

Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Abstracts Tuesday

Tu1 A 8.30-9.15

Novel Layered Nanomaterials: Controlled Synthesis, Electronic Properties and Applications

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Thermolytic routes to BC_2N and CN_x nanotubes will be presented. In particular, pyrolysis of $CH_3CN{\cdot}BCl_3$ over cobalt substrates at 950-1000 ºC leads to ca. BC_2N nanofibres and nanotubes exhibiting various morphologies. These structures have been investigated, at the nanometer level, using high spatial resolution electron energy-loss spectroscopy (HREELS). The presence of C-BN-C sandwich structures was observed within the 'graphitic' walls. This segregation processes may promote the formation of quantum dots or nanotube heterojunctions, which could then be used as nanotransistors operating high temperatures. Particular attention will be focused on efficient self-assembly pyrolytic routes to large arrays (2.5 cm^2) of aligned CN_x nanotubes/nanofibers (15-80 nm od and < 100 microns length). These 'hollow' fibres do not easily break upon bending and may behave as shock absorbing fillers in the fabrication of robust composites. Other novel applications will also be presented. These N-doped nanostructures have also been studied using tunnelling spectroscopy. Novel production routes to WS_2 and MoS_2 nanotubes will be presented. It will be shown that WO_x nanowhiskers behave as efficient templates of long WS_2 nanotubes after sulfidisation in the presence of H_2S. Additionally, MoS_2 nanotubes have been generated when polycrystalline MoS_2 powder, covered by Mo foil, is heated to 1300 ºC in the presence of H_2S. Finally, Density-Functional-based Tight-Binding (DFTB) calculations on MoS_2 and WS_2 nanotubes will be presented. They predict that all nanotubes observed experimentally (>20Å OD) should be semiconductors with a small band gap (lower than the bulk material). In addition, the electronic structure of novel metallic nanotubes of NbS_2 will be discussed.

Tu1 B 9.15-10.00

Optical Properties of Fullerene- and Non-Fullerene-Peapods

H. Kataura[1], T. Kodama[1], K. Kikuchi[1], K. Hirahara[2], K. Suenaga[2], S. Iijima[3], W. Kraetschmer[4], S. Suzuki[1] and Y. Achiba[1]

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[3] *Meijo University and NEC Corporation*
[4] *Max-Planck-Institute*

We realized high-yield fullerene-encapsulations in single-Wall carbon nanotubes. We confirmed a yield of encapsulation strongly depends on the mean diameter of nanotubes. Raman analysis shows a filling rate of C_{70}-peas is higher than 50% for 1.36 nm SWNTs in mean diameter, but less than 25% for 1.2 nm one. These results are consistent with the latest theoretical calculation. In this paper, we will discuss about optical properties of molecules encapsulated in nanotubes and of nanotubes encapsulating molecules to see interactions between them. In case of C_{60}-peas, the highest symmetric molecule, electron diffraction and resonance Raman spectra indicate spontaneous formation of C_{60} oligomers inside nanotubes. In the slightly lower symmetric C_{70} case, electron diffraction analysis indicates anomalously high-density packing instead of oligomers. These results can be explained simply by high-pressure state induced by a large potential energy gain via van der Waals interactions between fullerenes and nanotubes. Additionally, in the case of C_{70}, considerable modification of optical absorption and Raman spectra were observed. These are probably caused by less symmetric structure of C_{70} than C_{60}. On the other hand, the effects of encapsulation on nanotubes are not so large, such as slight up-shifts of radial breathing modes and the narrowing of energy gaps, very similar to the bundle effects. However, in case of the other molecule which has a similar size to fullerenes, vibrational properties of nanotubes were strongly affected by encapsulated molecules probably due to the less symmetric structure of the molecule.

Tu2 A 10.30-11.15

The Optical Properties and Electronic Structure of SWCNT: Empty, Stuffed or Surrounded by Dopants

M. S. Golden[1], X. Liu[1], T. Pichler[1,2], M. Knupfer[1], J. Fink, D. Walters[3], M. J. Bronikowski[3], R. E. Smalley[3], H. Kataura[4], O. Jost[5], A. A. Gorbunov[5] and W. Pompe[5]

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We present recent data concerning the investigation of the electronic structure and optical properties of SWCNT using electron and optical spectroscopies. Results will be discussed from aligned, pristine SWCNT, alkali metal intercalated nanotubes as well as from peapods which are nanotubes endohedrally doped with C_{60}. In addition, aspects of the understanding of the growth mechanism of SWCNT which can be derived from the systematic optical absorption study of the laser evaporation synthesis route will be discussed. This work was supported by the DFG, SMWK and the EU's IST Programme. T.P. is grateful to the ÖAW for financial support.

Tu2 B 11.15-12.00

Molecule/SWNT Interactions: Effects on Electronic and Phonon Properties

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The geometrical form of ropes of single Wall carbon nanotubes (SWNT) presents many opportunities to study experimentally for the first time the effects of adsorbed gases/molecules on the carbon pi electron system. These opportunities stem from the high symmetry of the nanotube, our fundamental understanding of the C-C interactions, the high specific surface area (m2/g) and the quasi-one dimensional nature of the ropes. We will present a wide ranging set of experimental results to probe the Molecule/SWNT interaction, including electrical transport (resistivity, thermopower), Raman scattering and gas storage measurements. Electrical transport studies indicate that we can distinguish between chemisorption and physisorption of various molecular species. We find the electrical properties of mats of SWNT ropes are sensitive to even gases like N2, H2 and He. Giant transport effects are observed for many organic vapors such as alcohols and aromatic molecules, leading us to propose that applications of SWNTs as a thermoelectric "nanonose" may be possible. The effects of many of these same adsorbed molecules on the Raman-active phonons of SWNTs have also been observed. Interesting shifts in the radial breathing modes are detected even though no charge transfer is suspected between the SWNT and the adsorbed molecules. These effects have been studied as a function of several molecular properties, e.g., polarizability, size, etc. Finally, we present results of large wt% hydrogen storage at crogenic temperatures in ropes of SWNTs, and we connect these results with theoretical estimates of the SWNT/ H2 interaction parameters.

Tu3 A 13.30-14.15

Chemistry of Single-Walled Carbon Nanotubes

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Most work on carbon nanotubes [CNTs](both single-walled and multi-walled), has been carried out on the usual intractable, insoluble form of the material. This form of the material is not amenable to many of the processing steps that are necessary if the CNTs are to reach their full potential – particularly in applications that require these materials in the form of polymers, copolymers, composites, ceramics and moldable forms. We have developed a procedure for the preparation of single-walled carbon nanotubes (SWNTs) that are soluble in organic solvents (s-SWNTs). This allows us to treat the s-SWNTs as macromolecules and to apply many of the techniques of organic and high polymer chemistry; in addition we can characterize the s-SWNT semiconductors and metals with standard solution spectroscopic methods. We have demonstrated both ionic (charge transfer) and covalent solution phase chemistry with concomitant modulation of the SWNT electronic band structure. Reaction of the s-SWNTs with dichlorocarbene led to functionalization of the nanotube walls. Gel permeation chromatography allows the purification of the s-SWNTs. Our work is directed toward the application of carbon nanotubes in materials science and biomedicine through solution processing and chemical modification of these materials. I will describe our latest results in this area.

PoS Tu1 14.15-17.30

Fluorinated Single-Wall Carbon Nanotubes

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Single-Wall carbon nanotubes (SWNTs) were synthesized by co-evaporation of graphite and cobalt-nickel ultra-disperse power during arc-discharge process. The content of SWNTs in the soot collected on a nickel screen was estimated from transmission electron microscopy (TEM) to be about 20%. The nanotube-contained material was fluorinated at room temperature using a volatile BrF_3. The elemental composition of sample produced was determined using X-ray photoelectron spectroscopy (XPS) to correspond to $CF_{0.1}$. Taking account that the soot is not fluorinated at applied synthetic condition and the tube content in the sample, the SWNTs are fluorinated up to C_2F composition. TEM showed that upon the fluorination the SWNT ropes are split into the individual tubes. Treatment of the product by hydrazine allows removing the fluorine. Conductivity of pristine, fluorinated, and defluorinated materials was measured by four-point technique. Fluorination lowers the room temperature conductivity of the samples more than in 10^4. The temperature behavior of conductivity for the fluorinated SWNTs was found to differ from that in the pristine material and to be characteristic of narrow-gap semiconductors. The defluorinated sample showed the increase of electron emission in the low-voltage region of I-V dependence compared to the pristine SWNTs.

PoS Tu2 14.15-17.30

Properties of Fluorinated Single-Walled Carbon Nanotubes as Derived from Density Functional Computations

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Fluorination of single-walled carbon nanotubes at elevated temperatures results in the production of tubular species with a stoichiometry close to C_2F. We here present the electronic and geometric structures of fluorinated single-walled nanotubes (F-SWNT) as obtained using density functional theory in conjunction with all-electron Gaussian basis sets under periodic boundary conditions. We find that the fluorine atoms are bound covalently to the tube surface, and that the band structure of the F-SWNT depends decisively on the distribution of the fluorine atoms. For certain fluorination patterns, metallic properties of the F-SWNT are expected. The geometries of the tubes distort significantly upon fluorination, e.g., resulting in pentagonal, tetragonal or trigonal structures for (5,5), (4,4), and (3,3) F-SWNT's, respectively. The mean C-F bond dissociation energy (BDE) increases with decreasing tube diameters; an interpretation of this behaviour is given. Comparing the C-F BDE with that of well known carbon-fluorine compounds indicates that the C-F bonds in small diameter F-SWNT are about as strong as those in graphite fluoride $(CF)_x$. Finally, the ^{19}F nuclear magnetic properties of F-SWNT and $(CF)_x$ are compared and discussed.

PoS Tu3 14.15-17.30

SWNTs Modified by Selective Nanoparticle Attachment

Y.Fan, S.Kooi, U.Schlecht, M.Burghard, K.Kern

Max Plank Institute for Solid State Research

Chemical modification of carbon nanotubes is an active field of research with the goal of tuning the tube's electrical or optical properties for various applications including ultrasmall electronic devices and chemical sensors. Here we report on two different approaches to modify single-walled carbon nanotubes by the attachment of nanoparticles. In the first case, selenium nanoparticles with sizes on the order of 10nm are selectively formed on the tubes upon treatment with H_2Se gas. The second approach involves modifying the tubes with a functional nitrene, created by photochemical activation. Sulfur group within the covalently attached residues can be used to bind different types of pre-formed nanoparticles (eg. Au, CdSe) with sizes in the range of 2-10nm. Both systems were analyzed by AFM, TEM, and EDX.

PoS Tu4 14.15-17.30

The Chemistry of Single Walled Carbon Nanotubes

Michael Holzinger and Andreas Hirsch

Institute of Organic Chemistry, Henkestr.42, Erlangen, Germany

In SWNT chemistry two types of derivatization are in principle possible: the amidation or esterification of the carboxylic acid groups of oxidized SWNT material and adding reactive groups onto the sidewalls. For derivatization of the carboxylic acid groups a large variety of methods are described (e.g. activation of the carboxyls by $SOCl_2$, DCC and EDC). In contrast, the reactivity of the sidewalls has received very little attention. From the chemist's point of view, SWNT sidewalls appear to be an intermediate form between graphite and fullerenes. On the one hand, the curved π-system of the exohedral region should have an increased electron density compared to planar graphite. On the other hand, having a diameter of about 1.4 nm the moderate curvature should result in less nucleophilic reactivity at the annealed benzene rings than found in C_{60}. For functionalisation of the SWNT sidewalls special reagents are required which exhibit pronounced reactivity. The reactions of C_{60} with nitrenes, carbenes and radicals have been described in detail. Here we present similar types of reaction with SWNTs prepared by arc discharge.

PoS Tu5 14.15-17.30

Theoretical Investigation on the Insertion of Li^+ into Carbon Nanotubes

Tapas Kar, J. Pattanayak and S. Scheiner

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Theoretical investigations have been carried out to explore the possibilities of Li ion intercalation or insertion through the side-Wall of single-Wall carbon nanotube. Hartree-Fock, MP2 and density functional theories with minimal to extended basis sets were used to estimate the potential energy surface (PES). The barrier to insert Li ion through these rings depends on the ring size. Insertion is easier as the ring size increases. Li ions favors two positions: a) inside the tube closer to the Wall, and b) outside of the tube. Atomic charge distributions/redistribution in different location of Li+ of the tubes are discussed.

PoS Tu6 14.15-17.30

Electrochemical Modification of Carbon Nanotubes

S. Kooi, Y. Fan, U. Schlecht, M. Burghard, K. Kern

Max Planck Institute for Solid State Research

The controlled electrochemical modification of individual single Wall carbon nanotubes (and small bundles) on Si/SiO_2 substrates is presented. The reduction of a diazonium salt in an aprotic solvent is employed to produce a radical that attacks the nanotube, forming a covalent bond between the nanotube and the dye molecule. In our experiments, the same nanotubes (bundles) were characterized by atomic force microscopy before and after modification. The possibility of using the attached dye molecule to bind a nanocrystal of choice (e.g. Au, Pt, CdSe) is explored. To achieve this goal, appropriate functional groups are produced by further electrochemical reduction of precursor groups on the dye.

PoS Tu7 14.15-17.30

Electronic Structure of Pristine, Fullerene-Filled and Intercalated SWCNT from High Resolution EELS in Transmission

X. Liu[1], T. Pichler[1,2], M. Knupfer[1], M. S. Golden[1], J. Fink[1], D. Walters[3], M. J. Bronikowski[3], R. E. Smalley[3], and H. Kataura[4]

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We present recent studies of the electronic structure and optical properties of SWCNT using high resolution electron energy-loss spectroscopy (EELS) in transmission. Firstly, we report the role of the SWCNT diameter upon the basis of data from SWCNT with mean diameters ranging from 0.8-1.4nm. We then discuss the effects brought about by doping these systems, either endohedrally with C_{60} molecules (forming so-called peapods) or exohedrally with alkali metals (n-type doping) or $FeCl_3$ (p-type doping).

PoS Tu8 14.15-17.30

Synthesis of Soluble Single-Walled Carbon Nanotube Derivatives

E. Menna[1], F. Della Negra[1], M. Cavallaro[1], M. Maggini[1], G. Scorrano[1], M. Meneghetti[2], F. Paolucci[3], M. Battagliarin[4]

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Most studies on single-Wall carbon nanotubes (SWNT) are physical investigations of solid state properties, while the chemical manipulation of nanotubes is still hampered by their insolubility and their extremely low reactivity. Some different approaches have been reported so far to the problem of bringing nanotubes to solution, such as pristine nanotubes suspension, inclusion in polymer matrices, sidewall functionalization. The approach we followed, reported by Smalley and coworkers [1] and by Haddon and coworkers [2,3], is based on the shortening of SWNT by means of an oxidative cutting process. Carboxylic functions formed at the edges can be conveniently used for further functionalizations. Here we report the synthesis and characterization of a SWNT derivative bearing poly(ethylene glycol) (PEG) chains that shows solubility in polar and non polar organic solvents. The product has been characterized by Raman spectroscopy, IR, NMR and some preliminary studies have been performed to evaluate photophysical properties, EPR and electrochemical behavior in solution. 1. J. Liu et al. *Science* **1998**, *280*, 1253-1256. 2. J. Chenet al. *Science* **1998**, *282*, 95-98. 3. M. A. Hamon et al. *Advanced Materials* **1999**, *11*, 834-840,786.

PoS Tu9 14.15-17.30

Nanoring Formation by Ring-Closure Reactions of Carbon Nanotubes

M. Sano, A. Kamino, J. Okamura, S. Shinkai

Chemotransfiguration Project - JST

Ring-closure reactions were applied onto single-walled carbon nanotubes in solution so that one end of a tube reacted with another end of its own. From the size distribution of nanorings, elastic properties in solution are analyzed.

PoS Tu10 14.15-17.30

Reversible Water-Solubilization of Single-Walled Carbon Nanotubes by Polymer Wrapping

Michael J. O'Connell, Peter Boul, Lars M. Ericson, Chad Huffman, Yuhuang Wang, Erik Haroz, Kevin D. Ausman, and Richard E. Smalley

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Single walled carbon nanotubes have been solubilized, primarily as individual tubes, in water by associating them robustly with linear polymers, most successfully with polyvinyl pyrrolidone and polystyrene sulfonate. This association is characterized by tight, relatively uniform association of the polymers with the sides of the nanotubes. A general thermodynamic drive for this wrapping is discussed, consisting of disruptions of the hydrophobic interface between each nanotube and the surrounding solvent, and of the smooth interaction surface in the bulk solid. These nanotubes can be recovered from their polymeric wrapping by changing their solvent system. This solubilization process opens the door to solution chemistry on pristine nanotubes, as well as their introduction into biologically relevant systems.

PoS Tu11 14.15-17.30

Raman Imaging of Chemically Modified Individual Carbon Nanotubes

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In this paper we will show that scanning confocal Raman microscopy can be used as an analytic tool to localize and investigate individual tubes and detect their vibrational modes with sub-mm lateral resolution. In particular, we present a detailed correlation of spectroscopic investigations and the geometry of thin bundles and individual single-Wall CNTs using scanning confocal Raman microscopy and scanning force microscopy. By using different excitation wavelength it is possible to mainly address the metallic or semiconducting tubes within a given bundle. Also, this approach allows to compare the Raman signals from chemically modified and unmodified CNTs. By subsequent deposition of oxidized and unoxidized CNTs, the different species can be clearly distinguished from one another and the effect of the oxidation upon the electronic structure can be investigated in detail.

PoS Tu12 14.15-17.30

Charge Transfer in Potassium Doped C_{60} Peapods from Resonance Raman Scattering

T. Pichler[1,2], W. Planck[1], A. Grüneis[1], H. Kuzmany[1], H. Kataura[3], Y. Achiba[4]

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We report on recent resonance Raman and resistivity measurements on potassium intercalation compounds of mats of fullerene containing SWNT (C_{60} peapods). In situ potassium intercalation results in an increased conductivity and a loss of the resonance enhancements of the modes of the SWNT due to a bleaching of the optical transitions. The radial breathing mode (RBM) of the doped SWNT is hardened and has only a small photon energy dependence. For the tangential modes the C_{60} A_g pinch mode has a well known frequency dependence on the charge transfer and on dimerization and polymerization. Following this relation for potassium intercalation of C_{60} peapods at low doping the charge transfer is predominantly to the SWNT whereas for full intercalation also charge transfer to the encapsulated C_{60} up to C_{60}^{-6} is observed. Work is supported by the FWF projects P12924 and P14146 and the TMR Research Network 'FUNCARS' (HPRN-CT1999-00011) from the EU. T.P thanks the ÖAW for funding.

PoS Tu13 14.15-17.30

Raman Studies of Alkali-Doping of SWNT

J.-L. Sauvajol, N. Bendiab, A. Zahab, E. Anglaret

G.D.P.C, Université Montpellier II

Phase transitions and staging in intercalated single Wall carbon nanotubes (SWNT) are controversial issues. In this communication, we report on combined in situ conductivity and Raman measurements of Rb doping of SWNT. Concomitant decrease of the resistance and change in the Raman spectrum are evidenced upon doping. In the last steps of doping, two distinct Raman spectra are observed and assigned to the Raman signatures of two different doped phases. These results are compared with Raman spectra recorded on SWNT sample doped with various alkali metals (Cs, Li, Na) at different and controled stoichiometries. All these results are discussed in terms of charge transfer and structural organisation in SWNT- alkali system. An unified interpretation of the whole results is proposed.

PoS Tu14 14.15-17.30

Visible Emissions of Single-Walled Carbon Nanotubes Formed in Zeolite Crystals

N. Nagasawa [1], I. Kudryashov [2], and Z. K. Tang [3]

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Mono-sized, aligned and single-walled carbon nanotubes (SWCNs) of about 0.4 nm diameter are formed inside micro-channel array of a zeolite single crystal. Since they are forced to align along c-axis of the crystal, they show strong polarization anisotropy in the optical absorption from near infrared to visible region [1]. The crystal is opaque in the polarization configuration E//c , but is almost transparent in E?c , where E is the electric field vector of the incident light. We have found strong emissions in visible regions under the monochromatic photo-excitations at room temperature. They showed strong polarization correlation with the absorption spectra. To know the spatial distribution of the emission sources and the origins, 3D micro-tomographic measurements are performed using the "Nanofinder" of nano-scale spatial resolution [2]. In this paper, we discuss these polarization characteristics in view of the selection rules of relevant optical transitions on the basis of the band calculation obtained by the LDA. [1] Z.K.Tang, Z.M.Li, G.D.Li, N.Wang, H.J.Li and C.T.Chan, to be published in the Proceedings of Inter. Symposium on Network Materials: Fullerenes, Nanotubes, and Related Systems, ISNM2001, Kamakura, Japan. [2] N.Nagasawa, I.Kudryashov, S.Tsuda, and Z.K.Tang, to be published in the Proceedings of ISNM2001.

PoS Tu15 14.15-17.30

Gas Adsorption Property of Single-Wall Carbon Nanohorns

K. Murata, K. Kaneko, D. Kasuya, K. Takahashi, F. Kokai, **M. Yudasaka** , and S. Iijima

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Single-Wall carbon nanohorns formed from single graphene sheets construct aggregates that have a large surface area. Porosity characteristics of the aggregates are similar to those of activated carbons, but the SWNH material does not need the high temperature and/or chemical treatment to activate itself. The pore sizes of the SWNH aggregates are controllable by selecting the duration and temperature of treatment in oxygen atmosphere. Such an easy control of pore-sizes is impossible for the conventional activated carbon. The pore-size control enables selective adsorption/storage of gas molecules.

PoS Tu16 14.15-17.30

Xenon Adsorption on the Outer Surface of Closed Ended SWNT Bundles

S.Talapatra, N.Dolan and A.D.Migone

Department of Physics, Southern Illinois University at Carbondale

Adsorption isotherms of Xenon on closed ended SWNT were measured in order to determine the adsorption behavior of this gas on the outer surface of the bundles. We will present monolayer adsorption data measured at various temperatures on nanotube samples from two different sources. The pressures at which Xe adsorption occurs on the highest binding energy sites on the SWNT's are lower than those for Xe on planar graphite, indicating that the binding energies for Xe are higher on the SWNT's. We will also present preliminary results for argon adsorption measurements on SWNT's.The Ar and the Xe results will be compared to each other and to results of computer simulations for these gases.

PoS Tu17 14.15-17.30

STM Study of a Grain Boundary in Graphite

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In a STM investigation of HOPG, an intriguing coiled structure was observed near a grain boundary. The atomic resolution obtained on this structure revealed a regular linear pattern parallel to the grain boundary. Theoretical simulations were elaborated in order to explain this characteristic pattern. They suggested that it could fingerprint a line of pentagon-heptagon couples resulting from Stone-Wales deformations of the hexagonal lattice close to the grain boundary.

PoS Tu18 **14.15-17.30**

Application of Partitioned Real-Space Density Functional Method to Field Evaporation from Carbon Nanotubes

N. Nakaoka, K. Tada, and **K. Watanabe**

Department of Physics, Science University of Tokyo

Recently, some carbon cluster ions have been selectively observed by field evaporation from carbon nanotubes [1].) When the electric field (the direction is opposite to that of electron field emission) is applied to the carbon nanotube tip, a carbon atom or cluster of the tip are positively ionized and evaporated toward the vacuum along the potential slope caused by the electric field. It has been impossible from first-principles calculations based on the density functional theory (DFT) to study the field evaporation under bias voltage (unequal Fermi energies) and zero electric current, because the DFT seeks the global ground state with one Fermi energy accompanying artificial electron transfer. To overcome the essential difficulty of the DFT above, we have developed a new partitioned real-space density functional (PRDF) method [2]) which determines the electronic states and two Fermi energies of bielectrode under bias voltage self-consistently. We applied the PRDF method to field evaporation from single-walled carbon nanotubes. We determine the potential energy curve for evaporation of C_5^+ cluster ion and found a drastic decrease in the activation barrier for evaporation in an electric field of 3V/A. The stable structure of the smallest fullerene ion, C_{20}^+, has been obtained. The details of the mechanism of field evaporation will be discussed. [1] K. Hata, et al., Chem. Phys. Lett. 308, 343 (1999). [2] N. Nakaoka, et al., Phy. Rev. Lett. 86, 540 (2001).

PoS Tu19 14.15-17.30

Iron Catalyst Chemistry in High Pressure Carbon Monoxide Nanotube Reactor

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The high-pressure carbon monoxide (HiPco) technique for producing single Wall carbon nanotubes (SWNT) is analyzed using a chemical reaction model coupled with properties calculated along streamlines. Streamline properties for mixing jets are calculated by the FLUENT code using the k-e turbulent model for pure carbon monoxide. The HiPco process introduces cold iron pentacarbonyl diluted in CO, or alternatively nitrogen, at high pressure, ca. 30 atmospheres into a conical mixing zone. Hot CO is also introduced via three jets at angles with respect to the axis of the reactor. Hot CO decomposes the $Fe(CO)_5$ to release atomic Fe. Cluster reaction rates are from Krestinin, et al., based on shock tube measurements. Another model is from classical cluster theory given by Girshick's team. The calculations are performed on streamlines that assume that a cold mixture of $Fe(CO)_5$ in CO is introduced along the reactor axis. Then iron forms clusters that catalyze the formation of SWNTs from the Boudouard reaction on Fe-containing clusters by reaction with CO. Time histories of temperature and dilution that were calculated by the fluid dynamics code FLUENT are inputs for simulating the chemical process along streamlines. Alternative catalyst injection schemes are also evaluated.

PoS Tu20 14.15-17.30

Hydrogen Storage Mechanism in Single-Walled Carbon Nanotubes

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A novel mechanism of hydrogen storage in carbon nanotubes is proposed by using the density functional calculations. Several key intermediate states are identified for hydrogen adsorption. Up to the coverage of 1.0, hydrogen atoms chemisorb on the nanotube Wall with either an arch type or a zigzag type. Then, hydrogen can be further stored inside the nanotubes at higher coverage as a molecular form. Hydrogen atoms can be inserted into the nanotubes through the tube Wall via flip-in and/or kick-in mechanism with activation barriers of 1.5 and 2.0 eV, respectively. In the hydrogen extraction process, hydrogen molecules inside a nanotube firstly dissociates onto the inner Wall with an activation barrier of 1.6 eV. Secondly, hydrogen atoms at the interior of the tube Wall are further extracted to the outer Wall by the flip-out mechanism with an activation barrier of 2.0 eV. Our theoretical calculations support the experimental observations of electrochemical hydrogen storage in nanotubes.

PoS Tu21 14.15-17.30

Tribo-Effects in Nanotubes

Petr Král

The Weizmann Institute of Science

I discuss new tribo-effects in nanotubes, as induced by light and friction with fluids. First, I complement our recent work [1], showing that atoms intercalated in C nanotubes can be driven by a dc electric current, which is generated optically by mixing one and two-photon interband electron transitions. In particular, I show [2] that in heteropolar BN nanotubes, monochromatic laser beam can generate electric currents of orientations controlled by the structure of nanotubes. These currents are accompanied by ultrafast mechanical expansions of the BN nanotubes. Finally, I show that electric currents can be induced in metallic nanotubes immersed in flowing liquids [3]. Here, the friction between molecular layers and the nanotube generates an asymmetrical flow of phonons in the nanotube, which can drag free carriers. These new phenomena have potential photo-electric and photo-mechanical applications. I discuss also other photo-effects in nanotubes, which we have studied recently. [1] P. Král and D. Tománek, Phys. Rev. Lett. 82, 5373 (1999). [2] P. Král, E. J. Mele and D. Tománek, Phys. Rev. Lett. 85, 1512 (2000). [3] P. Král and M. Shapiro, Phys. Rev. Lett. 86, 131 (2001).

Abstracts Wednesday

We1 A 8.30-9.15

Carbon Nanotube and its Application to Nanoelectronics

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The application of carbon nanotube to nano electronics, especially for the high-density memory device and the display application have been reviewed. There have been reported that carbon nanotube can be applied for the field effect transistor and nonvolatile memory device. The prototype carbon nanotube based field emission display with low power consumption and high brightness has been demonstrated. In order to make realization of the carbon nanotube on the market, several factors have to be considered. The controllable properties, selective growth, nano-device design, connection, circuit interfacing must be achieved together with higher performance than the conventional device. In this presentation, the feasibility of carbon nanotube to the nano electronics and recent progress of our research will be discussed.

We1 B 9.15-10.30

Carbon Nanostructures: Growth, Electron Emission, Interactions With Hydrogen

Louis Schlapbach*, Oliver Gröning, Pascal Ruffieux, Lars-Ola Nilsson, Patrick Sudan, Philipp Mauron, Christophe Emmenegger, Pierangelo Gröning, Andreas Züttel

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We grow carbon nanostructures on pretreated substrates in view of their use as electron source or as electrode for supercaps and study the interaction of various forms of condensed carbon with hydrogen. The reaction of atomic hydrogen with sp2-type graphitic carbon in the planar, 1D-curved nanotubes and 2D-curved fullerenes, respectively, is clearly different as it evolves from photemission studies.
Results on the reversible sorption of molecular hydrogen gas by single walled and multiwalled carbon nanotubes are still not very promising: the amount of physisorbed/desorbed hydrogen is roughly proportianal to the specific surface area, for nanotubes as well as for nanostructured graphite made by intense ball milling. When absorption conditions are changed to higher temperatures to allow dissociation of hydrogen, mass spec controlled thermal desorption clearly shows that hydrocarbons were formed. A rigorous control of nanotube growth and clear physical and chemical characterisation is needed prior to make final conclusions.
High specific surface area carbon is reached upon nanotube thin film growth; the films are suitable as electrodes for electrochemical doublelayer capacitors.
Fowler-Nordheim type electron emission occurs at low electric fields of the order of 2-3 V/mm due to local field enhancement. Fluctuations of the emission site and of the emission current are observed. Conceptionally simple electron sources working around room temperature seems to be an attractive application; again rigorously controlled growth is needed. We discuss effects of the statistical distribution of the local field enhancement factor.

We2 A 10.30-11.15

Inorganic Nanotubes and Inorganic Fullerene-Like Materials of Metal Dichalcogenides

Reshef Tenne

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Much progress has been achieved in the synthesis of inorganic nanotubes and fullerene-like nanoparticles of WS_2 and MoS_2 over the last year or two. Synthetic methods for the production of multiwall WS_2 nanotubes by sulfidizing WO_3 nanoparticles have been described and further progress is underway. A fluidized-bed reactor for the synthesis of 20-50 g of fullerene-like WS_2 nanoparticles has been reported. The detailed mechanism of the synthesis of fullerene-like MoS_2 nanoparticles has been elucidated. The construction of a reactor for the production of ca. 1 g of such nanoparticles is in progress. Substantial progress has been achieved in the use of such nanoparticles for self-lubricating mechanical parts. It was shown that, impregnation of 3-8 wt% of these nanoparticles in various porous matrices, produced self-lubricating parts with a reduced friction, a higher load bearing capacity and extended lifetime expectancy. It has been indicated that slow release of the nanoparticles from the porous matrix to the matting surfaces and the high lubricity power of such nanoparticles are responsible for the improved tribological properties of such nanocomposites. Applications for such nanocomposites will be described.

We2 B 11.15-12.00

CVD Synthesis of Single Walled Carbon Nanotubes on Aerogel Supported Catalysts

B. Zheng, Y. Li, M. Su and **J. Liu**

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Among all methods currently used for Single-walled carbon nanotube (SWNT) synthesis, chemical vapor deposition (CVD) method represents the best hope for large-scale production. We have synthesized SWNTs using metal catalysts supported on aerogel supports. The yield of nanotube prepared with uniform amount of catalyst is significantly improved. The yield and quality of the produced nanotubes depend on many important factors, including the surface area, chemical composition of the aerogel support, type of catalyst, size of catalyst particles, feed gas etc. Systematic studies have been performed to understand the effect of these factors and to optimize the experimental conditions to prepare SWNTs with high quality and high yield.

We3 A 13.30-14.15

Theoretical Studies of Quantum Transport, Pyro- and Piezo-Electric Effects and Lithium Intercalation

J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, C. Roland, and Q. Zhao

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We have investigated the electronic and quantum transport properties of bent, deformed and tapered nanotubes, as well as nanotube-metal contacts, which will likely form components of future nanotube-based devices. Bent armchair nanotubes keep their metallic character up to fairly high angles, while metallic chiral nanotubes open a sizable gap at the Fermi level, indicating that they can be used as nanoscale strain sensors. Tapered armchair tubes remain metallic, while their zigzag counterparts are semiconducting, as expected. Ballistic transmission is very sensitive to interactions with the substrate and coupling to the contacts. Our *ab initio* calculations for NT/Al structures show substantial charge transfer and rehybridization effects, which strongly affect the quantum conductance. We have also investigated BN nanotubes that are intrinsically polar. For BN tubes in chiral or zigzag structures, the symmetry permits a pyroelectric field along the tube axis, which is of the order of kV/cm per nanotube. The pyro- and piezo-effects will likely be useful in nanoscale switches, resonators, actuators, and transducers. Turning to Li intercalation in carbon nanotubes, we have shown that Li cannot penetrate nanotube walls unless 9-fold rings or larger openings are present. Our large simulations Li motion lead to aggregation in the interstitial channels.

We3 B 14.15-15.00

Carbon Nanotube Molecular Wires: Recent Progress in Synthesis, Characterization and Devices

Hongjie Dai

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I will first briefly review our work in controlled growth of multi-walled and single-walled carbon nanotubes with ordered structures on surfaces. The general growth approach involves chemical vapor deposition of hydrocarbons on patterned substrates by supported catalyst as well as individual nanoparticles. I will then show that the controlled growth readily leads to nanowire device structures useful for characterization of the fundamental properties of nanotubes and potential applications. With these devices, we have carried out systematic measurements of the electrical, mechanical and electromechanical properties of nanotubes. Since nanotubes are unique electronic materials with every atom exposed at the surfaces, surface issues are critical to the physical properties of nanotubes. We have elucidated the interactions between nanotubes and molecular and metal species, and carried out non-covalent functionalization of nanotube sidewalls with small molecules and proteins. The potential of nanotube molecular wires as ultra-small chemical and biological sensors will be discussed, and the latest results of chemical gating effects and nanotube-based sensing will be presented.

PoS We1 15.30-18.30

CVD Grown Carbon Nanotube Tips for Atomic Force Microscopy

V. Barwich, R. Bennewitz, **A. Baratoff** and E. Meyer

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Small-diameter, high-aspect ratio, stiff, but highly flexible carbon nanotubes (CNT) are well-suited for Atomic Force Microscopy (AFM). We can grow thin individual CNT on the pyramidal tip of a microfabricated silicon cantilever. Catalyst particles (alumina enclosed by iron and molybdenum or a thin film of iron) are first deposited and then subjected to CVD. The optimal parameters for growing thin, straight CNT are about 750°C, 10 min and 10:700:1050 cm^3/min for a ethylene-hydrogen-argon mixture. Suitable protruding CNT were characterized by SEM, then shortened to less than 200 nm by electrical etching in order to reduce the lateral thermal vibration amplitude. Images of ionic crystal surfaces have been recorded in UHV in the non-contact mode. Resonance frequency vs. distance curves reveal the desired reduction of long-range forces.

PoS We2 15.30-18.30

Symmetry Principles of Friction – Nanotubes

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The symmetries of two compounds significantly affect their interaction. This is sublimated within three basic principles, which are applied to the carbon nanotubes (finite and infinite) to explain recently proposed [1] and observed [2] low friction effects. The friction decreases on account of the symmetry breaking mechanism, which can produce even the super-slippery interaction: the Goldstone mechanism makes that the walls in an infinite incommensurate double-Wall nanotube freely slide. As a general recipe for lubricant selection, the results may be of interest in tribology. [1] M. Damnjanovic, I. Milosevic, T. Vukovic and R. Sredanovic, Phys. Rev. B **60** (4) (1999) 2728. [2] John Cumings and A. Zettl, Science, **289** (2000) 602.

PoS We3 15.30-18.30

Hollow Nanoparticles of WS_2 as Superior Solid Lubricant

L. Rapoport, V. Leshzinsky, I. Lapsker, M. Lvovsky, Yu. Volovik, R. Rosentsveig, Y. Fedman and **R. Tenne**

Holon Academic Institute of Technology and the Weizmann Institute of Science

Recently, inorganic hollow nanoparticles of metal dichalcogenide MX_2 (M=Mo,W,etc.;X=S,Se) with structure related to nested carbon fullerenes and nanotubes (designated inorganic fullerene-like materials - IF) have been developed. It has been shown that IF possess superior lubricating properties over solid lubricants with lamellar structures, like graphite and MoS_2 (2H platelets). We attribute the recently reported outstanding tribological behavior of IF-WS_2 to its chemical inertness and to the hollow cage structure, which leads to high elasticity and allows the particles to roll rather than slide (rolling friction) in appropriate loading regimes. Unfortunately, the slippery nature of these nanoparticles leads to their fast displacement from the contact area, and consequently the efficacy of their lubrication is maintained so long as they can be replenished to the contact area. By confining the IF nanoparticles inside a porous and densified solid matrix, prepared by powder metallurgy (PM) techniques, slow release of the IF nanoparticles onto the metal surface alleviates both friction losses and wear, while assuring the mechanical integrity of the composite. A multiscale tribological model is proposed, according to which the nanoparticles reside in the pores and are furnished to the surface where they serve as both a lubricant and spacer. The potential ramifications of this work for self-lubricating bearings, gears, etc. are also discussed.

PoS We4 15.30-18.30

Scaling Laws for Van der Waals Interaction of Hollow Nanoparticles

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We present theoretical investigations of the effect of van der Waals interactions on crystal properties, phase behavior and adhesion properties of hollow nanoparticles made from layered material like C or WS_2. Since the van der Waals interaction scales linearly with radius R, the heat of sublimation is larger than for molecular scale van der Waals solids. Since the interaction range between particles scales inversely with R, the gas-liquid coexistence disappears from the phase diagram for particle radii in the range of 1-3 nm (depending on Wall thickness h). Upon van der Waals adhesion to a substrate, both nanospheres and nanotubes can deform considerably, albeit with different scaling laws in regard to R and h.

PoS We5 15.30-18.30

A New Hybrid Nanocomposite Formed by Intercalation of Multi-Walled Carbon Nanotubes into Epoxy Swelled Montmorillonite Clay

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Mechanical reinforcement of polymers using randomly oriented Multi-walled Carbon Nanotubes (MWCNT) has shown limited benefits due to localized polymer matrix strain. To overcome this difficulty we investigated combinations of MWCNT and ion exchanged montmorillonite layered silicates in an epoxy polymer. Mechanical reinforcement was examined using Dynamic Mechanical Spectroscopy. Similar dispersion problems are expressed by MWCNT and layered silicates due to charge mediated flocculation. Dispersion was achieved using an organic electron donor solvent. Particle surface interaction then took place at the bound surfactant on the silicate platelet. Intercalation of MWCNT between the layered silicates was imaged using Scanning Electron Microscopy (SEM). The connected fiber architecture was shown to mitigate polymer strain damage by nanotubes. Particle orientation in the hybrid composite was observed on curing in a 6kV electric field. This demonstrated that control of the hybrid composite microstructure was possible to further develop strength, damage resistance, fracture toughness, and polymer film barrier properties.

PoS We6 15.30-18.30

Synthesis and Characterization of Single-Walled Carbon Nanotubes/Polymer Network Composites

H. Goering, H.-E. Maneck, U. Knoll, S. Gajewski, K.-W. Brzezinka, R. Mach, H.-D. Klotz, A. Schönhals, J.F. Friedrich

Bundesanstalt f? Materialforschung und -pr?ung, Unter den Eichen 87, Berlin, D-12205, Germany

Blending of a flexible polymer matrix and a nanoscopic rod-like filler is an important method to improve the mechanical and electrical properties of polymer materials. For a mechanical reinforcement the effect is increased with the concentration, the aspect ratio and the modulus of the filler. However, the improved electrical conductivity of the systems needs the percolation of the filler particles. Considering both aspects carbon nanotubes are an ideal nanoscopic material for blending polymers. Single-walled carbon nanotubes (SWNT) used in this work were synthesized by dc arc discharge process using metal-doped graphite anode (Ni/Y=4/1 at.%). The as grown SWNTs have been purified by chemical methods using HCl to remove catalyst particles followed by oxidation with HNO_3. This purification process was controlled by TGA, SEM, TEM and Raman scattering. The SWNTs were dispersed in the monomer component before the polymer network was formed. The dispersion process was assisted by surfactants. The synthesized SWNT/epoxy resin and SWNT/polyurethane network composites were characterized by TEM, SEM, DMA, Raman scattering, and dielectric relaxation spectroscopy. For establishing structure-properties relationship, specific mechanical and electrical parameters are discussed. As expected, concentrations of SWNT smaller than 1 wt.% influence strongly these properties of the polymer matrix as well as the structure of the networks.

PoS We7 15.30-18.30

Carbon-Nanofibre-Filled Thermoplastic Composites

Jan Sandler[1], Milo Shaffer[1], Jacek Nastalczyk[2], Christian Keun[2]

[1] *Department of Materials Science and Metallurgy, University of Cambridge, UK*

Experimental and theoretical results suggest that carbon nanofibres (CNF) hold promise as reinforcement materials for novel nanocomposites. We have investigated a range of composite systems using nanofibres of differing structure and diameter in a number of representative thermoplastic matrices, including commodity and high performance resins. We have particularly examined mechanical and electrical properties of the nanocomposite materials and, as with conventional composites, have found that the critical factors influencing composite performance are quality of the nanofiller, the nature of the filler dispersion, and the strength of the filler-matrix interface. We have achieved a high degree of dispersion in all matrices, using an intensive shear mixing protocol in conventional thermoplastic processing equipment, and have fabricated standard test samples by injection moulding. The degree of dispersion can be monitored directly by electron microscopy and by analysis of the dielectric response. Microscopy, mechanical testing, and micro-Raman studies have shown that the interfaces between untreated nanofibres and the thermoplastic matrices tested are very weak and little or no load is transferred to the filler. Use of a pre-oxidation treatment, however, can increase the interfacial bond strength, leading to an increase in stiffness and yield strength for certain systems.

PoS We8 15.30-18.30

Electronic and Mechanical Properties of Hydrogen Functionalized Carbon Nanotubes

Liu Yang, Richard Jaffe, Jie Han

NASA Ames Research Center

We examined the electronic and mechanical properties of hydrogen functionalized carbon nanotubes. The functionalization pattern covers two extreme groups. One group has randomly selected functionalization sites including one to twenty percent of the carbon atoms. The other group has regularly patterned functional sites parallel to the tube axis. Metallic, small-gap semiconducting and large-gap semiconducting carbon nanotubes are studied. The results reveal that the electronic properties of the tubes are very sensitive to the degree of functionalization, with even one percent functionalization being enough to render metallic tubes semiconducting. On the other hand, the mechanical properties, like tensile modulus, are much less sensitive to functionalization. For carbon nanotubes functionalized with specific patterns, the electric properties depends strongly on the nature of the functionalization pattern.

PoS We9 15.30-18.30

Simultaneous Determination of Inclusion Crystallography and Nanotube Conformation for a Sb_2O_3:SWNT Composite

S. Friedrichs, R.R. Meyer, J. Sloan, A.I. Kirkland, J.L. Hutchison, M.L.H. Green

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The detailed inclusion crystallography of a 1-dimensional valentinite Sb_2O_3 crystal incorporated within a helical (21,-8) single walled carbon nanotube has been identified from a phase image that was recovered via a modified object wave restoration scheme. A detailed analysis of asymmetric fringe contrast in the tube walls has provided strong evidence for the chiral sense of the tube itself. Due to the good agreement of observed Wall periodicity with the determined absolute focus values and power spectra obtained from single-pixel line traces along both tube walls, we were able to determine the chiral sense of the SWNT and the tilt angle of the Sb_2O_3/SWNT composite relative to the electron beam. The angle between the optimum <1 0 -1> viewing direction of the crystal fraction and the tube axis, which is aligned with the <4 -1 2> direction of the Sb_2O_3 crystal, is 78.3°. Since small deviations from this viewing direction make an insignificant difference to the observed contrast, a tube inclination of 15° is plausible for both the Sb_2O_3 crystal and the assigned (21,-8) SWNT, which is the mirror image of a (13,8) SWNT.

PoS We10 15.30-18.30

BN and B/N-Doped C Nanotubes: Synthesis, Structure, Properties and Applications

Dmitri Golberg and Yoshio Bando

National Institute for Materials Science

Multi-walled nanotubes made of B/N-doped C and pure BN were synthesized through thermo-chemical treatments of CVD-grown multi-walled C nanotubes, boron oxide and various metal oxide promoters in a flow of nitrogen at 1700-2000 K using high-frequency induction currents. Nanotube structure and B, C, N atom species distribution were analyzed using a JEM-3000F field emission 300 kV electron microscope equipped with a Gatan 2D-DigiPEELS electron energy loss spectrometer and an energy dispersion X-ray detector, and an Omega filter JEOL-3100 field emission 300 kV electron microscope. Preferential "zigzag" chirality and unique rhombohedral-like stacking between tubular shells were first observed in the BN-rich nanotubes. New approaches for making exclusively open-ended tubes and synthesizing BN nanotubes with definitely preferred even number (2, 4) of tubular shells were developed. In addition, B/N-doped C and BN tube filling with discrete metal clusters or metal nanowires was first carried out. Energy filtered TEM images allowed to discover peapod-like structures in B/N-doped C and BN tubes, existence of heterojunctions between BN-rich and C-rich nanotube domains, and complex nanotubular ropes extending up to several micrometers in length, and composed of C-rich and BN-rich tubes. Nanotube formation mechanism, structural models, thermal and chemical stability, and prospects for technological applications will be discussed in the presentation.

PoS We11 15.30-18.30

Structural Stability and Electronic Structure of Boron Nanotubes

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After the recent discovery of superconductivity in a new class of inorganic compounds, metal-intercalated boron analogues of graphite, we decided to address the existence of nanotubes, made up of boron in a honeycomb structure, similar to carbon nanotubes. Using first-principle total-energy methods, we investigated the structural stability of some boron nanotubes, and found them to be metallic by band-structure calculations. The cohesion of the bare boron tube is relatively poor, but its bending strain energy is comparable to those of C and BC analogues. Then we investigated the effect of the insertion of metal atoms inside the nanotubes. While magnesium does not seem strongly stabilized, we found that a constructive interaction occurs with aluminum atoms, which strongly stabilize the structure of the smallest boron nanotubes.

PoS We12 15.30-18.30

BN Substituted Carbon Compounds: A Theoretical Study

Tapas Kar, J. Pattanayak and S. Scheiner

Department of Chemistry and Biochemistry, Utah State University, Logan, UT 84322-0300

Previous theoretical and experimental investigations on B/C/N systems are mostly concentrated on 50:50 combinations of C and BN units, i.e., BC_2N stoichiometry. In the present theoretical investigation we will replace one by one pair of carbon atoms by isoelectronic BN unit. Successive replacement patterns, structure, stability, nature of bonding and electronic properties of such hybrid materials are discussed.

PoS We13 15.30-18.30

Vanadium Oxide Nanotubes as Cathode Materials in Rechargeable Lithium Batteries

Kristina Edström, Sara Nordlinder, Torbjörn Gustafsson, Jun Lu and Eva Olsson

Departments of Materials Chemistry and Analytical Materials Physics, The Ångström Laboratory, Uppsala University, SE-751 21 Uppsala, Sweden

Vanadium oxide in the form of scroll-like nano-rolls is here demonstrated as a cathode material for rechargeable lithium batteries. The rolls consist of several vanadium oxide layers, separated by structure-directing agents (templates). Two different types of nanotubes, one with hexadecylamine ($C_{16}H_{33}NH_2$) and another with dodecylamine ($C_{12}H_{25}NH_2$) as templating molecules have been studied. In addition, the effect of Na+-exchange on the microstructure of the latter is analysed. By the use electrochemical techniques, *in situ* X-ray diffraction, electron spectroscopic imaging and high angle annular dark field imaging, a picture of the internal structure of the tubes and its function as a cathode material have evolved. The battery performance is shown to be closely dependent on type of lithium salt used in the electrolyte. The highest capacity (>200 mAh/g) is found using Na+-exchanged material and an electrolyte containing $LiN(SO_2CF_3)_2$ as the lithium salt. The nano-rolls can be charged/discharged at least 100 cycles with preservation of the tubular structure. Details of the tubular structure and lithium insertion/extraction mechanisms will be discussed in the light of the performance as battery material.

PoS We14 15.30-18.30

Carbon Nanotube Based Composites as Electron Injection Layers in Organic Light Emitting Diodes

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Organic light emitting diodes have been fabricated, incorporating carbon nanotube based composites as electron injection layers. At moderate nanotube loading levels, electron injection into M3EH-PPV was increased by over three orders of magnitude. This was accompanied by a substantial increase in electroluminescent efficiency. This is explained by improved current balance leading to higher singlet exciton yield.

PoS We15 15.30-18.30

Systematic Study of Carbon Nanotubes Static Polarizabilities as a Function of Radius, Length and Helicity

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Electron field emission by carbon nanotubes has very attractive properties for potential industrial applications such as flat panel displays. Its low turn-on field can be interpreted partly by the very high field enhancement at the tip of the nanotube. This enhancement can be linked to the nanotube polarizability. Previous studies on that subject used a tight-binding approximation for infinite length nanotubes (Benedict et al. Phys. Rev. B 1994, 52, 8541) or dipole-dipole interactions between the carbon atoms, for finite length nanotubes [(5,5) and (9,0)], with an isotropic carbon polarizability (Jensen et al., J. Phys. Chem B, 2000, 104, 10462) . We present here the results of a systematic study of carbon nanotubes static polarizabilities, using a dipole-dipole interaction model with anisotropic carbon polarizabilities, derived from graphite (P. Senet, Kirchberg 1993 ; M. Devel et al., Phys. Rev. B, 1996, 53, 13159). We show that the polarizabilities parallel and perpendicular to the tube axis are quadratic and linear functions of length, respectively, for fixed indices. Then, we study the influence of the radius on the previous proportionality coefficients, for a fixed helicity, and finally the influence of helicity. The resulting empirical laws can be used to predict the parallel and perpendicular polarizabilities of a wide class of single-Wall carbon nanotubes.

PoS We16 15.30-18.30

Field Enhancement Properties of Carbon Nanotubes

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Flat panel displays represent a very promising technological application of field emission from carbon nanotubes films, thanks to their low turn-on field. One mechanism suspected to lead to this property, is the polarization of the nanotube in the applied field leading to a high enhancement of the field. We have therefore studied the evolution of the field enhancement factor for various single-Wall, double-Wall and triple-Wall nanotubes, by means of a self-consistent resolution of Poisson's equation in a dipolar approximation (Ch. Adessi et al., Phys. Rev. B, 2000, 62, R13314). Large differences between the β factor of (n,0) and (n,n) nanotubes are observed. Actually, a saturation of the field enhancement with the length of the tube is observed for (n,n) nanotubes conversely to (n,0) nanotubes which can lead, for small diameter nanotubes, to very high value of the β factor as observed experimentally. Moreover, we have verified, in the case of multi-Wall nanotubes, that the inner shell holds up its field enhancement property. Finally, the effect of the nanotube density on the field enhancement is reported for a nanotubes film.

PoS We17 15.30-18.30

Field Emission from Individual Carbon Nanotubes: Towards a High-Brightness Electron Source

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Carbon nanotubes (CNTs) are not only of interest for fundamental studies, but also for a range of practical applications. One such potential application is using a CNT as an electron source in high-resolution electron beam instruments, such as electron microscopes. The key requirements for such a source are high brightness, small energy spread, and stability. Gaining insight in the relation between the material properties of CNTs and their performance as an electron source, demands the investigation of individual nanotubes. We are studying a wide variety in CNTs, such as multi-walled, single-walled, metallic, semiconducting, open-ended and closed. To this end, we perform experiments on field emission from individual carbon nanotubes mounted on tungsten tips. We have measured energy spectra, current-voltage characteristics, and angular emission distributions. The energy spectra are particularly helpful in characterizing the nanotubes, and may yield information that distinguishes between metallic and semiconducting behavior. Measurements of energy width and stability have already shown results that are promising for applications. Second, we are studying the brightness of individual CNT field-emitters using point-projection microscopy. In addition, we are currently exploring several different mounting, preparation and characterization techniques of our nanotube samples. Our latest results will be presented at the workshop.

PoS We18 15.30-18.30

MOCVD Approach to Aligned Isolated Carbon Nanotubes. Materials for Cold Cathode Field Emitters

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Carbon nanotubes (CNTs) are promissing materials for cold cathode field emitters [1]. Parallel alignment over large areas has to be achieved to reach this goal. We have studied organic as well as organometallic catalytically driven template based thermal CVD approaches to achieve this goal [2,3]. These Approaches are attractive due the single source strategy used wich employs the use of low cost organometallic complexes containing both the metal as well as the carbon atoms [4]. Geometric structuring of the alumina embedded CNTs can be achieved either by a laser structuring process or by simple ink jet catalyst impregnation [5]. By using organometallic precursors a single source strategy is possible wich even allows to incorporate metals within the CNTs. In situ visualisation of the individual field emission sites was achieved by field emission spectroscopy. [1] P. Calvert, *Potential Applications of Carbon Nanotubes*, in *"Carbon Nanotubes, Preparation and Properties"* (T.W. Ebbesen, ed.), CRC Press, Boca Raton, USA, **1997**. [2] G. Che, B.B. Lakshmi, C.R. Martin, E.R. Fisher, *Chem. Mater.* **1998**, *10*, 260. [3] J.J. Schneider, G.L. Hornyak,et al., *Nanostr. Mater.* **1999**, *12*, 83. [4] C.N.R. Rao et al., *Chem. Commun.* **1998**, 1525. [5] J.J. Schneider, J. Engstler et al., *Chem. Eur. J.* (2001) *in press*.

PoS We19 15.30-18.30

Field-Dependent Secondary Electron Emission from MgO-Deposited Carbon Nanotubes

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A highly enhanced secondary electron emission from MgO-deposited carbon nanotubes under a large bias voltage has been found recently by a collaborating experimental group and its underlying mechanism is investigated in the present work. We propose a self-consistent semi-classical model based on a major redistribution of charge to explain a huge amount of secondary electrons and their energy distribution which deviate from the standard theory of secondary electron emission. We analyze the effects of the primary electron energy, bias voltage, and the thickness of MgO on the yield of secondary electrons, and they are compared with the experimental data. Ab initio pseudopotential electronic structure calculations are also performed for the MgO-deposited tubes to help clarify the basic mechanism. Critical factors for a large yield of emission and their significance to practical applications will be discussed.

PoS We20 15.30-18.30

Field Emission Energy Distribution for an Undergated Triode CNT-FED

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We have measured I-V characteristics and field emission energy distribution (FEED) for an undergate-type triode carbon nanotubes-field emission display (CNT-FED), which has gate electrodes with an insulating layer located under the cathode electrodes. The emitters of an undergated CNT-FED were fabricated by the printing method with CNT paste, which was mostly consisted of glass powders. For the diode emission, the FEED peaks (E-EF) shift with 67 meV/V, and ? was found to be 26,054 ?-1 from the I-V measurement. On the while, peaks for the triode emission shift with 270 ~ 500 meV/V because of the strong electric field induced by the gate. We also observed subpeaks below the main peaks, which may be occurred from the existence of glass surrounding CNTs. The FWHM of peaks for diode and triode emission were broader than those reported by others, i.e., 0.7 ~ 1.9 eV, which may be caused by field emission from various geometry of CNTs. In summary, we measured the FEED of the undergated CNT-FED for the first time, and the FEED peaks shift as the applied voltage increased, which supports the energy band bending in CNTs.

PoS We21 15.30-18.30

Growth and Properties of CVD-Grown Carbon Nanotube Films

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Films of carbon nanotubes are technologically interesting, for example as cold cathodes in field emission devices. We grow such films directly onto substrates by thermal chemical vapour deposition, employing the catalytic activity of iron particles which are produced in situ. Films of aligned and non-aligned carbon nanotubes can be synthesised, depending on growth conditions and on the type of carbon precursor molecule used. In this contribution we discuss the various nanotube film morphologies and nanotube structures which are obtained when hydrocarbon or fullerene molecules are used as carbon feedstock gases. Film characterisation is carried out by electron microscopy and Raman spectroscopy, and the correlation between these two methods is demonstrated. Our results show how the diameter distribution of the supported catalytic metal particles influences the formation of nanotubes and other carbon structures. We also perform field emission measurements on various as-grown nanotube films which enable us to correlate nanotube film structure information to field emission effiencies. The field emission process is accompanied by a strong light emission, which is spectrally analysed.

PoS We22 15.30-18.30

Oxidation in Air of CCVD and Laser-Ablation Carbon Nanotubes

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The aims of the study of the oxidation in air of CNTs samples are to characterize the samples on a macroscopical scale, by detection of the phases that may be present (SWNTs, MWNTs, nanocapsules, ...), to purify the sample by selective oxidation and to investigate the opening of CNTs tips. Laser-ablation (Tubes@Rice) and CCVD (the authors laboratory) specimens are studied by DTA and TGA/DTG in isothermal and non-isothermal modes. Their specific surface area is measured. Selected specimens are observed by HREM. The laser-ablation sample is oxidized in two steps (355 and 450°C) corresponding to the amorphous carbon and residual surfactant and to the SWNTs bundles, respectively. For the CCVD CNTs, there is a competition between the oxidation of SWNTs and that of outer walls of DWNTS and TWNTs. In the as-prepared CNTs-Co-MgO powders, some CNTs tips are opened, then the outer Wall of DWNTs is oxidized (up to 420-440°C), leading to an increase in the proportion of SWNTs. In the corresponding extracted CNTs, SWNTs are oxidized below 400°C, then the DWNTs and TWNTs are opened and eventually oxidized. The difference could arise from the more compact nature of the extracted sample. The interpretation of the DTA patterns will be discussed.

PoS We23 15.30-18.30

Scroll-to-Nanotube Transformation: The Zipper Mechanism

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Using total energy calculations, we investigate the relative stability of multi-Wall nanotubes and graphitic scrolls, as well as a possible conversion in-between these structures. We show that scroll segments, consisting of rolled-up graphite sheets, may coexist with segments consisting of nested tubes within a single tube, separated by a dislocation region. Energy considerations suggest that such dislocations may easily be created at the elevated temperatures during nanotube formation. We also propose a bond-rearrangement mechanism that allows an axial zipper-like motion of the dislocation, thus converting a scroll into a multi-Wall nanotube segment, or vice versa. Due to the low energy cost of the zipper motion, and in view of the instability of a scroll with two unsaturated edges along the axis, we find that a scroll-to-nanotube conversion is energetically favorable and may proceed even at room temperature, unless hindered by defects.

PoS We24 15.30-18.30

Scrolls and Nested Structures in Multiwalled Carbon Nanotubes

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Since multi-walled carbon nanotubes (MWNT) were discovered about a decade ago there has been considerable interest in their structural intricacies, growth mechanisms, and electrical and mechanical properties. The tips and closure structures of MWNT have been the topics of intense scrutiny. Recent analysis of defect structures along the tube walls shows that most MWNT are complex structures composed of scroll-like and nested features existing side-by-side. Within the nested tubes, helicity changes little from layer to layer, and depends only on layer diameter. Such an analysis should lead to a better understanding of the unique properties of carbon nanotubes.

PoS We25 15.30-18.30

Transformation of Single-Wall Carbon Nanotube Ropes into Multiwall Carbon Nanotubes

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Recently it has been discovered that bundles of single-Wall carbon nanotubes (SWCNT's) transform into multiwall carbon nanotubes (MWCNT's) under thermal treatment at high temperatures (2300 K-2500 K). The MWCNT's produced by such a transformation contain from 2 to 6 nested tubes. To investigate this "showy" structural transformation of the tubes, from SWCNT ropes into MWCNT's, we have performed extensive molecular dynamics (MD) simulations using semiempirical potentials to mimic the Carbon-Carbon interactions. We propose a possible mechanism for this transformation based on the "concerted" coalescence of the tubes in the bundle. The roles played in the structural transformation by the size of the tubes as well as by their chiralities are analyzed.

PoS We26 15.30-18.30

Hydrogen Storage in Carbon Nanotubes: A Neutron Scattering Investigation

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Carbon single-walled nanotubes (SWNTs) were prepared by pulsed laser vaporization and cleaned by annealing in dynamic vacuum. Both, as prepared material consisting of closed SWNTs and chemically treated material consisting of opened SWNTs were charged with hydrogen gas at 180 bar. Inelastic Neutron scattering data including raw spectra, the phonon density of states and the dynamical susceptibility (quasielastic component) will be presented for different temperatures between 150 K and 400 K. Clear evidence is obtained for larger amounts of H_2 adsorbed inside the SWNTs giving rise to a well pronounced inelastic scattering spectrum which reaches up to »250 meV. Most of the weakly bond H_2 desorbs rapidly near 300 K however, tightly bond hydrogen is still observed at higher energies and 400 K. Structural information on both kinds of materials as obtained from elastic and quasielastic scattering contributions will be discussed. By a comparison to a Vanadium standard we can quantify our results

PoS We27 15.30-18.30

Application of Carbon Nanotubes to Energy Storages

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Carbon nanotubes have been intensively investigated for their fundamental and technical importances. Several issues for the applications to energy storage of hydrogen storage, secondary battery, supercapacitors will be discussed. Hydrogen storage using hydrostatic pressure and electrochemical approaches with carbon nanotubes are currently on debate. The maximum storage capacity reported so far varies from group to group. We will demonstrate that the storage capacity is strongly dependent on the sample-preparation conditions. The stability, flatness on the voltage scan, and cycle life will be extensively discussed. On the other hand, the supercapacitor with non-fadadaic reaction has long cycle life and high power density but low energy density. Therefore development of a supercapacitor with high energy density is always desirable. We demonstrated already a maximum capacitance of 180 F/g and a measured power density of 20 KW/kg and an energy density of 7 Wh/kg in a solution of 7.5 N KOH using singlewalled carbon nanotubes [1]. These values are still lower than that of commercially available activated carbons. We will report our effort to improve the energy density using various nanotube-polymer composites.

PoS Su28 15.30-18.30

Curvature and Hybridization Effects in Carbon Nanotubes

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The curvature effects in carbon nanotubes are studied analytically as a function of chirality. The β-orbitals are found to be significantly rehybridized in all tubes, so that they are never normal to the tubes' surface. This results in a curvature induced gap in the electronic band-structure, which turns out to be larger than previous estimates. The tilting of the β-orbitals should be observable by atomic resolution scanning tunneling microscopy measurements.

PoS We29 15.30-18.30

Ab Initio Calculation of the Absorption and Energy-Loss Spectra of a Bundle of Carbon Nanotubes

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The frequency-dependent dielectric response function, optical absorption and energy-loss spectra (EELS) have been calculated for a solid of (5,5) armchair carbon nanotubes. We have started from a DFT-LDA ground state calculation using norm-conserving pseudopotentials. The spectra were then obtained in the random phase approximation (RPA) and in the time-dependent local-density approximation (TDLDA), including local field (LF) effects. The response function and spectra were determined for different polarizations and wave-vectors of the exciting light or electrons. Both LF and the polarization are expected to be important for nanotubular structures which possess a high degree of structural inhomogeneity and anisotropy. We discuss our findings in the light of recent theoretical calculations and experimental observations (EELS, optical absorption) of single-Wall (SWNT) and multi-Wall (MWNT) nanotubes and nanotube bundles.

PoS We30 15.30-18.30

Plasmon Excitations in Isolated SWCNT

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Optical conductivity tensor for isolated single-Wall carbon nanotubes (SWCNT) of arbitrary chirality is found. The calculation is based on the maximally reduced tight binding method [1] and dipole approximation. The line group symmetry of the SWCNT [2] is taken into account and the matrix elements of the momentum operator are calculated exactly. The result is used to interpret the EELS measurements of the tubes with the same radii showing different behaviours (almost doubled intensity and 3 eV peak position shift) [3]: the effect is related to the parities of the electronic states and strongly depends on the polarization of the perturbing field. The interpretation can be used to complete the identification of the geometrical structure of the tubes under study. [1] M. Damnjanovic, T. Vukovic, I. Milosevic, J. Phys. A **33** (2000) 6561. [2] M. Damnjanovic, I. Milosevic, T. Vukovic and R.Sredanovic, Phys. Rev. B **60** (4) (1999) 2728. [3] T. Stöckli, Ph. D. Thesis, Lausanne, EPFL (1999).

PoS We31 15.30-18.30

Dynamics of Low Energy Optical Excitations in SWNTs: Cooling of a Laser Heated Electron Gas and Non-Equilibrium Effects

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We present a time-domain study of the relaxation of electronic excitations in SWNT- and HOPG-samples at lattice temperatures between 40 K and 320 K. Time-resolved photoemission is used to probe the dynamics of the optically excited electron gas. A detailed analysis of the Fermi-edge in the photoelectron spectra is used to determine the increase and lowering of the electron-gas temperature after optical excitation of the sample by a visible femtosecond laser-pulse. The cooling of the electron-gas is intimately related to the coupling of electrons to lattice vibrations and can be used to measure the electron-phonon coupling strength. Such energy transfer between electrons and lattice may also contribute to current induced failure in SWNTs. We find that the observed temperature decay at different lattice temperatures is consistent with dominant electron-lattice energy-transfer by back-scattering from longitudinal acoustic phonons. Certain features in the photoemission spectra, however, cannot be attributed to the dynamics of a thermalized electron gas and indicate a dynamic shift of the electrochemical potential. The magnitude and direction of this shift can be related to the sample density of states and derivative at the Fermi level.

PoS We32 15.30-18.30

Light Emission from Carbon Nanotubes

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Carbon nanotubes have been synthesised on Si substrates by use of Hot Filament assisted CVD (HFCVD) technique. Typical synthesis parameters were a 5 - 15 vol. % methane proportion in hydrogen, a 1800 - 2000 °C filament temperature and a 700 - 900°C substrate temperature. The growth morphology observed with SEM and crystallographic structure determined by TEM demonstrated that depending on substrate preparation and synthesis conditions MWNT or SWNT have been prepared. Thanks to Raman spectroscopy measurements undertaken for different laser radiations (633nm, 514 nm and 458 nm), the presence of very well crystallized and pure SWNT has been demonstrated. Moreover, emission lines due to recombination of electron-hole pairs at different Van Hove singularities have been recorded in semiconducting SWNT. This suggests significant potentiality of these novel materials for optoelectronics applications.

PoS We33 15.30-18.30

Transport and Magnetic Properties of Brominated Multiwall Carbon Nanotubes

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Laminated carbonaceous material composed of multiwall carbon nanotubes has been prepared by arc discharge graphite evaporation in helium atmosphere. Scanning electron microscopy showed that the inner part of carbon deposit grown on the cathode consists of tubular particles mainly. The tubes were estimated by transmission electron microscopy to have from 2 to 30 shells with outer diameter of 60-150 A. The brominated material was prepared by exposure of the pristine one to Br_2 vapors. Its composition was determined by x-ray photoelectron spectroscopy to be $CBr_{0.06}$. The magnetoconductivity, magnetic susceptibility and temperature dependence of conductivity of pristine and brominated samples were investigated. The pristine sample was found to characterize by conductivity anisotropy 10^2, which disappears after sample bromination. The positive magnetoconductivity and additional contribution to magnetic susceptibility of the pristine material and the brominated material was observed. The extrinsic conduction carrier concentration n_0 for the pristine sample and brominated that was estimated in the framework of the quasi-two-dimensional graphite band model by the method of Kotosonov using the fitting parameters of diamagnetic susceptibility. Really, the value of n_0 for brominated sample increases in comparison to that for pristine sample from $3x10^{10}$ to 10^{11} cm^{-2}.

PoS We34 15.30-18.30

Nonlinear Optics of Intense Ultrashort Light Pulses in Carbon Nanotubes

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Carbon nanotubes (CNs) are characterized by strong nonlinearities which are yet not completely understood. The nonlinear optical properties make CNs attractive for different applications and are expected to provide useful information on the dynamics of electron motion in CNs. In particular the pronounced electronic nonlinearity in CNs could represent a useful mechanism for the generation of very short wave-lengths by high-order harmonic generation (HHG) in a device confined to a very small sub-mm region. In our contribution we present a quantum-mechanical theory of the nonlinear optical properties of CNs exposed to an intense ultrashort pulse. The theory takes into account the effect of interband transitions of p-electrons and utilizes a direct analysis in the time domain. We predict the current density harmonic spectrum as a set of discrete lines imposed by incoherent continuous background. Further we study the characteristic features of the third and fifth harmonics as well as of the harmonics of very high orders in metallic and semiconductor CNs and demonstrate a new cutoff mechanism for HHG. The results of the rigorous quantum-mechanical theory are compared with that of our previous semiclassical theory [1]. [1] G. Ya. Slepyan, et al., Phys. Rev. A61 R777 (1999); Phys. Rev. A63 (2001, accepted)

PoS We35 15.30-18.30

Adsorption Studies of Xenon on Carbon Nanohorns

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Adsorption isotherm measurements were performed on recently discovered nano-aggregates of graphitic nano horns (SWNH). The data suggests that there are two different groups of adsorption sites present in the substrate. The energy of the highest binding site was determined from low coverage adsorption isotherm data by calculating the isosteric heat of adsorption for nine (190 K - 305 K) different temperatures. The binding energy for these higher energy sites is 48% greater than that for Xe on planar graphite and 15% smaller than that of closed ended single walled carbon nanotubes (SWNT). Results of full isotherms, measured to determine the monolayer capacity of Xenon on SWNH sample, will also be presented.

PoS We36 15.30-18.30

Nanotube Sensors for the Detection of Failures Within Integrated Circuits

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GMA Industries, Inc.

This abstract describes original research and development in the use of nanotube-based chemical and electronic sensors as embedded test equipment within the architecture of integrated circuits (ICs) to detect failures that may affect IC reliability and performance. This R&D being performed by the Nanoteknology Division of GMA Industries, Inc., focuses on the monitoring of electrical and chemical activity within the IC to provide a fast, accurate, and inexpensive identification of failures. Results are presented from the development of two nanotube-based devices: a metal migration sensor and a nanotube rectifier diode. The metal migration sensor uses the properties of carbon nanotube conductivity to detect a small change in current density caused by an increased area in contact with the metal, while the overlapping of two semiconducting nanotubes creates the rectifier diode. We will describe our methods for the chemical modification and tailoring of nanotube properties to fulfill our application requirements, convey any experimental results achieved to date, and discuss lessons learned in the process.

PoS We37 15.30-18.30

Structural and Electronic Properties of a Carbon Nanotorus: Effects of Extended vs Local Deformations

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To study the effects of bending of a carbon nanotube, we consider a carbon nanotube bent into a ring and follow the deformation of a carbon nanotorus through various stages, namely, from elastic deformation to the onset of the kinks and eventually to the collapse of the walls of the nanotorus. The changes in the electronic properties due to extended deformations are contrasted with those due to local deformations to bring out the subtle issue underlying the reason why there is only a relatively small reduction in the electrical conductance in the former case even at larger bending angles while there is a dramatic reduction in the conductance in the latter case at relatively small bending angles.

PoS We38 15.30-18.30

Evaluation of the Mechanical Properties of Carbon Nanotubes and Nanofibres Under Hydrostatic Pressure by Laser-Raman-Spectroscopy

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Experimental and theoretical results suggest that carbon nanotubes (CNT) and vapour-grown carbon nanofibres (VGCNF) hold promise as reinforcement materials for novel nanocomposites. Although recent progress has been made in testing the mechanical properties of individual carbon nanotubes, a statistically significant experimental analysis of the stiffness of CNT and VGCNF as a function of structure remains a challenging task. In this study the mechanical properties of bulk samples of CNT and VGCNF from different production methods were analysed by Micro-Laser-Raman-Spectroscopy. During hydrostatic compression in a diamond anvil pressure cell the in-plane deformation of the graphitic planes was studied by following the characteristic 1580 cm^{-1} Raman peak (G band). It has been shown previously for macroscopic high-modulus carbon mesophase pitch fibres that the rate of the G band shift per unit strain is proportional to the Young's modulus. We demonstrate that the Raman peak shift as a function of hydrostatic pressure can be used to evaluate the elastic mechanical properties of a wide variety of nanoscale carbon materials. In addition, we demonstrate a discontinuity of the elastic response of the nanotubes and nanofibres which we attribute to a reversible flattening and finally an irreversible break down of their structure at high pressures.

PoS We39 15.30-18.30

A Neutron Scattering Investigation of the Pressure-Induced Structural Changes and Low Frequency Excitations in SWNT Bundles

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In a first part we investigate the pressure-induced structural changes of single-Wall carbon nanotubes organised into 2D crystalline bundles by neutron diffraction up to 50 kbars. The pressure dependence of the position of the (10) Bragg peak is found to depend on the orientation of the axis of the anvil cell with respect to the diffraction plane. This behavior implies the presence of an uniaxial pressure component along the axis of the anvil cell. The pressure dependence is well described in the framework of a pressure-induced progressive deformation of the tubes section, from circular to hexagonal, in addition of the van der Waals compression. In a second part we present recent inelastic neutron scattering measurements of the vibrational density of states (VDOS) of single Wall carbon nanotubes, by focusing in the low frequency range (E<12 meV). We report the first unambiguously evidence of low frequency excitations assigned to libration and twist modes of tube in bundles. A linear dependence of the VDOS in the range 0-1.5 meV was systematically observed in neutron experiments for SWNT samples prepared with various techniques. We discuss the main features of this density of states in the light of calculations using a force constant model including interactions up to the fourth neighbor in the tube and considering a van der Waals interaction between the tubes.

PoS We40 15.30-18.30

Hydrogen Adsorption on Different types of Nanotubes

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A key technological barrier to the development of fuel cells, particularly for portable and transportation uses, is the unavailability of a compact, high storage capacity, lightweight and rechargeable hydrogen storage system. The recently discovered Carbon Nanotubes are now the fastest-growing subfield of carbon materials research. The unique structure, physical and chemical properties of these recently discovered fullerene nanotubes materials have lead to the investigation of these materials for many applications. One potential application that has received significant research effort is that of hydrogen storage in these unique carbon structures. The method of production and associated characteristics of different types of carbon nanotubes (the different types of Single-walled, arc multi-walled, CVD random multi-walled CVD aligned multi-walled nanotubes) will be presented. The physical hydrogen adsorption capacities (gravimetric and volumetric) of all these different types of carbon nanotubes will be presented and discussed. Post treatment processing of the carbon nanotubes and its effect on their hydrogen adsorption will be presented. The results of hydrogen adsorption on the high purity aligned MWNT will also be presented and used as a model for the role of nanotubes in hydrogen adsorption.

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