SYMPOSIUM A
Nanotubes and Related Materials
November 27 – 30, 2000

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*Invited paper
SESSION A1: SYNTHESIS I  
Chair: Sumio Iijima  
Monday Morning, November 27, 2000  
Grand Ballroom (Sheraton)

8:30 AM #A1.1  
GROWING SINGLE-WALLED CARBON NANOTUBES IN THE GASPHASE. Petri Wilke, Michael J. Brzuskowski, R. Kelly Bradley, Dan La Cour, Robert H. Haynes, A. Smith, and Richard E. Smalley, Center for Nanoscale Science and Technology, Rice University, Houston, TX.

Large-scale production of high-purity carbon single-walled nanotubes (SWNTs) has been achieved via the High Pressure Carbon Monoxide (HiPCO) Process. This gas-phase process utilizes a continuously recirculating flow of highly pressurized (14100 atm) carbon monoxide as the feedstock gas for the nanotube production. Into a precisely-designed region at the heart of the apparatus, an approximately room temperature gas mixture containing ppm concentrations of metal carbonyls is rapidly mixed into a flow of hot (700-1100K degrees C) CO gas. Following thermal decomposition of the organometallic precursors, metal atoms condense into clusters entrained in the flowing gas. These clusters act as catalyst particles upon which SWNT nucleate and grow via CO disproportionation: CO + CO → CO2 + 2 C.

The resulting nanotubes are swept downstream of the mixing region and are collected on a series of filters. In this fashion, SWNT material of up to 99 mole-% purity has been produced at rates up to 350 mg/hr from a prototype laboratory reactor designed and fabricated at Rice. The dependence of the quantity and quality of SWNT material produced on system parameters such as temperature, pressure, and catalyst concentration/composition will be discussed, along with recent technical advances in the HiPCO experimental apparatus.

9:00 AM #A1.2  
PERFECTLY-ALIGNED SINGLE WALL CARBON NANOTUBE CRYSTALS. Jin Won Seo1,2, James K. Gimzewski2, Reto R. Schletter2, 1Institut de Physique, Université de Neuchâtel, Neuchâtel, SWITZERLAND; 2IBM Research Division, Zurich Research Laboratory, Holschwil, SWITZERLAND; Mark E. Welland, Engineering Department, University of Cambridge, Cambridge, UNITED KINGDOM.

Since the discovery of carbon nanotubes in 1991, [1], new methods of synthesizing multi-walled and single-walled carbon nanotubes (MWCNTs and SWCNTs, respectively) have been developed from the initial use of hot arc discharges, to laser ablation and more recently catalytic chemical vapor deposition and solid-state chemical reactions. SWCNTs are currently the subject of much research because they represent an ideal 1-D nanostructure with unique physical properties. Nevertheless, only limited success has been achieved in the preparation of ordered bundles [2,3], which are thought to be held together by weak Van der Waals forces. Here we demonstrate a new breakthrough where perfect single crystals made of well-ordered SWCNT bundles are directly fabricated using a nano-patterned metal oxide reaction in vacuum. Transmission electron microscopy (TEM), Atomic Force Microscopy and Electronic Loss Spectroscopy were used to characterize the structure and unique ordering of the tubes. Single-walled tubes within a single crystal were found to be in close contact and have uniform diameters of approximately 1.5 nm, which provides them with the unique capability to order in the micron scale. The bundles were found to terminate abruptly and they exhibit facetting, particularly in larger crystallites. Video sequences of aspects of the growth process using in-situ heating in the TEM will also be used to illustrate the basic growth mechanism. [1] Iijima, Nature 354 (1991) 56. [2] A. Thes et al., Science 273 (1996) 483. [3] Y. Zhang et al., Science 285 (1999) 1719.

9:15 AM #A1.3  
VECTORIAL GROWTH OF CARBON NANOTUBES. Ernesto Joselevich, Thomas Roeske, Kyoung Ha Kim, Charles M. Eicher, Harvard University, Department of Chemistry and Chemical Biology, Cambridge, MA.

Carbon nanotubes have been proposed as ideal interconnects for molecular electronics. Recently, for instance, a novel approach for carbon nanotube based random access memory has been presented. In order to realize these concepts, new methods are required for the production of ordered arrays of nanotubes on surfaces. Here we demonstrate a novel concept whereby the growth of carbon nanotubes on the surface is geometrically defined as a vector. Single-wall carbon nanotubes are produced by chemical vapor deposition on silicon wafers under the action of a local electric field parallel to the surface. The orientation of the vectorial growth is defined by the electric field. The mechanism of growth and field-orientation, and its implications are discussed.

9:30 AM #A1.4  
FORMING ALIGNED NANOTUBE INTERCONNECTIONS BETWEEN THIN Ni LAYERS AND Si(001). Bingqing Wei, Z.J. Zhang, P.M. Ajayan, and G. Ramaswamy, Department of MS&E, Rensselaer Polytechnic Institute, Troy, NY.

There is widespread interest in growing networks of aligned carbon nanotubes for creating new nanoscale device architectures on planar substrates such as Si. It is crucial to evolve strategies to interconnect nanotubes with each other, with catalytic metal films, and with Si layers on a single substrate, for realizing such architectures. Here, we demonstrate a way of growing vertically aligned nanotubes, which connect patterned metal lines and the Si substrate. Thin Ni layers were lithographically patterned on Si(001) substrates and exposed to xylene-methane mixtures. Electron microscopy of the exposed samples show that vertically aligned multiwalled nanotubes grow only underneath the Ni layers, and result in the lifting-off of the Ni patterns from the substrate. Thus, a forest of nanotubes links the Ni layer and Si(001).

In some areas, the delaminated Ni film flips over, without detaching from the nanotubes, indicating a strong bonding between Ni and the nanotubes. The mechanism of metal film lift-off and nanotube alignment are discussed in the context of the nanotube growth behavior on patterns of other metal alloys.

9:45 AM #A1.5  
SINGLE-WALL CARBON NANOTUBE SYNTHESIS BY THE ROOM TEMPERATURE IRRADIATION OF MILLISECOND CO2 LASER PULSES. Fumio Koki, Kunimitsu Takahashi, Institute and Research and Innovation, JAPAN; Daisuke Komiy, Meijo Univ., JAPAN; Masako Nishikawa, JST-I-CORP, JAPAN, and Sumio Iijima, JST-I-CORP, N.C, Meijo Univ., JAPAN.

Single-wall carbon nanotubes (SWNTs) were synthesized by the irradiation of CO2 laser pulses (1.2-20 ps pulse widths and 1 kW peak power) on a graphite-C60 composite target at room temperature in an argon gas environment. In this experiment, CO2 laser pulses obtained on a quartz tube wall in front of the target, the intensity of a beam is about 180 mW/cm2, due to the radial breathing mode of SWNTs, relative to that of a broad band at 1350 cm-1, due to non-SWNT carbon materials, was found to change significantly depending on the width of the CO2 laser pulse. TEM micrographs of the SWNTs synthesized by room-temperature CO2 laser irradiation showed thinner bundle structures, compared to the SWNTs synthesized with the help of a furnace (1200°C). In a-polar laser pulses produced by CO2 laser pulses with 1.2-20 ps pulse widths, emissions of C2 (Swan bands) and C3 and blackbody radiation was observed. The C2 and C3 emissions were distributed near the target (~2m from the target). However, the blackbody radiation was observed up to about 5 cm from the target. Based on the temperature distribution of the plume (C2 vibrational temperature and the temperature of clusters and particles estimated using Planck blackbody radiation function) and shadowgraphic images indicating the formation of mushroom and turbulent clouds of growing graphitic materials through the interaction of Ar gas, we discuss SWNT growth from a molten carbon-metal particle via supersaturation and segregation during the time of milliseconds.

SESSION A2: SYNTHESIS II  
Chair: Daniel T. Colbert  
Monday Morning, November 27, 2000  
Grand Ballroom (Sheraton)

10:30 AM #A2.1  
NANOTUBE CATALYST OPTIMIZATION USING COMBINATION APPROACHES. Alan M. Cassell, Sanita Verma, Goldwyn Parker II, Ramsey Stevens, Catienn Nguyen, Lance DeLisit, Meynya Meiyappam, Jie Han, NASA Ames Research Center, Moffett Field, CA.

Libraries of liquid-phase catalyst precursor solutions were printed on various substrates and evaluated for their effectiveness in catalyzing the growth of carbon nanotubes by chemical vapor deposition (CVD). The catalyst precursors were composed of inorganic salt solutions of Al, Si, Fe, Co, Ni, Mn and a removable tri-block copolymer structure-directing agent. Scanning electron microscopy (SEM) was used to rapidly screen the catalyst libraries for activity. Parameters such as catalyst composition (stoichiometry, concentration) and reaction conditions (temperature, gas flow rate) were varied to quickly identify high yielding nanotube catalysts. As many as 50 different catalysts can be screened at one time, making the discovery process much less time-consuming. Catalyst compositions were identified that afforded aligned multi-walled carbon nanotube arrays as well as high yielding, single-walled carbon nanotube arrays.
nanotube arrays. The optimized catalysts were then employed in a variety of applications such as the growth of probing microscope probes and nanoelectronic components.

11:00 AM A2.2
CONDUCTIVE PHASE CONVERSION GROWTH OF CARBON NANOTUBES D.B. Geoghegan, X. Fan, M.C. Guillen, R.D. Sears, S.J. Pennycook, Oak Ridge National Laboratory, Oak Ridge, TN; A.A. Puretzky, Department of Materials Science and Engineering, Univ. of Tennessee, Knoxville, TN.

Single-wall carbon nanotubes (SWNT) are efficiently grown by laser vaporization of composite carbon and metal catalyst targets inside a hot oven environment. From time-resolved, in situ imaging and laser spectroscopy of the vapor plume of vaporized material, along with TEM analysis of deposits collected under direct diagnostic monitoring, we conclude that the majority of SWNT growth occurs over seconds of time from a feedstock of carbon clusters and nanoparticles. By situ imaging of the rapid growth of "beads" and nanotubes in a condensation plume of SWNT, supporting a condensed phase conversion of particulate carbon feedstock by activated metal catalyst nanoparticles or SWNT "beads" as a viable mechanism for growth of carbon nanotubes during laser vaporization. These measurements have been broadened and extended to include the growth of multiwall carbon nanotubes by condensed phase conversion (CPC) of various feedstocks. The processing conditions resulting in optimal nanotube growth were monitored using in situ diagnostics and ex situ FEM and TEM analyses of the resulting carbon nanotube-based carbon composites.

11:15 AM A2.3
SYNTHESIS OF HOMOGENEOUS DIAMETER SINGLE-WALL CARBON NANOTUBES BY HIGH TEMPERATURE INDUCTION HEATING Thomas Geniet, Rochester Institute of Technology, Department of Materials Science and Engineering, Rochester, NY; Anne C. Dillon, Jeff L. Allen, Kim M. Jones, Phillip A. Parilla and Michael J. Heben, National Renewable Energy Laboratory, Golden, CO.

Over the past several years a large number of synthetic procedures for the production of Carbon Single-Wall Nanotubes (SWNTs) have been developed. The resultant SWNT materials, regardless of the specific synthetic technique, are a mixture of various diameters and types of SWNTs. The polydispersity in tube diameter and type makes it difficult to observe the physical, electrical and mechanical properties of specific nanotubes. Nanodisperse or “diameter-pure” nanotubes are required in order for a more detailed understanding of SWNT materials. This presentation will describe a set of experimental conditions utilizing induction heating of a graphite target that reproducibly results in the synthesis of a very narrow diameter distribution of SWNTs. Our typical synthesis technique is similar to the pulsed laser vaporization technique described by Guo et al [1]

Under a 100 cc/mn argon flow the susceptor is heated by inductively-coupled RF to a maximum of 1650°C as measured by a two color pyrometer. The maximum temperature is limited by the coupling of the induction heating supply to the susceptor. The rest of the reaction vessel is not externally heated. The resultant web-like material is collected and subsequently analyzed by Raman and optical spectroscopy as well as TEM. A very narrow diameter distribution corresponding to a Raman line centered at 182 cm⁻¹ is observed. The SWNTs also form unusually small bundles containing as few as 1-5 tubes. The results indicate that the high temperature of the target material coupled with the low temperature of the immediate surroundings greatly reduce the reaction phase region as the laser strikes the target. This rapid quenching produces an SWNT raw scoot with a very narrow diameter distribution and small bundle sizes. These results will be discussed in greater detail. [1] T. Guo, P. Nikolaev, A. Thess, D.T. Colbert and R.E. Smalley, Chem. Phys. Lett. 1995, 243, 49.

11:30 AM A2.4

Previous experimental results by in-situ diagnostic in pulsed laser ablation found atomic species or small clusters [C2, C3, C6] disappear during most of the single wall carbon nanotube (SWNT) growth period. Also the Z-contrast imaging and electron energy loss spectroscopy do not find any metallic atoms incorporated in the carbon nanotubes, and no carbene species smaller than 2 nm in diameters. Furthermore, continuation of growth was achieved outside the laser ablation chamber indicating a condensed phase growth mechanism. Therefore we propose a new atomic level nucleation and continuing growth theory for catalyst mediated SWNT growth. In this model, both carbon and catalyst are vaporized and condensed first forming metallic clusters followed by the metal catalyst condense on to the carbon clusters. The well established equilibrium bulk carbon/metal phase diagram suggests that they form either liquid or solid/liquid eutectics nanoparticles/droplet at high temperature. The further cooling leads to the phase separation in carbon/catalyst nanoparticle. With sufficient low carbon concentration and small particle size, the carbon atoms can diffuse fast enough to one side of the particle and form solid carbon phase. Theoretical studies show that carbon clusters are more favorable to form caps than the flakes when the atom number is 340. Although cage is more favorable for free carbon clusters, cap is more likely in this case because the presence of catalyst. The interaction between catalyst and carbon at the interface will determine the optimal diameter of the cap. Once the cap is formed, further carbon segregation is naturally occurring at the root of the cap which eventually leads to a cylindrical tube. Since no vapor phase carbon/catalyst is needed in this growth model, condensed phase continuing growth is readily achieved with high temperature of supplies of carbon atom.

11:45 AM A2.5
FORMATION OF CARBON NANOTUBES AND SILICON NANOWIRES BY RAPID THERMAL PROCESSING FROM ION-BEAM SPUTTERED FILMS T.S. Wang, K.H. Chen, Academia Sinica, Institute of Atomic and Molecular Sciences, Taipei, TAIWAN; L.H. Chen, National Taiwan University, Center for General Education Sciences, Taipei, TAIWAN; C.T. Wang and K.J. Ma, Chang Cheng Institute of Technology, Dept. of Mechanical Engineering, Long-Tan, TAIWAN.

We report here an efficient method to produce carbon nanotubes (CNT) and silicon nanowires (SiNW) using rapid thermal process (RTP) of thin films deposited by ion beam sputtering (IBS). Both RTP and IBS are convenient and robust techniques suitable for the growth of large-area wafer processes and are well established in the industry. For CNT, iron-containing amorphous carbon film was first prepared by IBS from graphite-Fe mixed target, then subjected to RTP for different duration times at temperatures of 800°C–1200°C. For SiNW, iron-containing amorphous Si film was first prepared by IBS from Si-Fe mixed target and followed by RTP treatment. The RTP treatment was carried out in either argon or nitrogen ambient at temperatures of 1100°C–1200°C. The resultant CNTs were found to be most efficient for transforming amorphous carbon into CNT. For instance, high density of multi-wall CNTs with a diameter of about 15-30 nm and a length of 500 nm were found to cover the entire substrate after RTP for 20 sec at 1200°C in nitrogen ambient. The IBS/RTP approach offers an unprecedented opportunity for studying the kinetics of CNT growth in that the dimension changes of CNT can be monitored as a function of time and temperature in a controllable manner.

SESSION A3: ELECTRONIC PROPERTIES I
Chair: Luc Henrard
Monday Afternoon, November 27, 2008
Grand Ballroom (Sheraton)

1:30 PM A3.1
FUNDAMENTAL PROPERTIES AND APPLICATIONS OF SINGLE-WALLED CARBON NANOTUBES Charles M. Lieber, Harvard University, Department of Chemistry and Chemical Biology, Division of Engineering and Applied Sciences, Cambridge, MA.

Single-walled carbon nanotubes (SWNTs) represent unique systems both for testing our fundamental understanding of the physics of low-dimensional materials and for building new nanoscale tools and devices. This presentation will overview selected studies addressing both aspects. First, atomically-resolved scanning tunneling microscopy and spectroscopy studies of the interaction of magnetic atoms and clusters with extended and finite size SWNTs, and the structure and electronic properties of intramolecular nanotube junctions will be described. Second, a new concept for a carbon nanotube molecular scale computer, which is based on a suspended SWNT crossbar array, will be discussed together with proof of concept experiments. Third, critical tools for imaging, sensing and manipulation at the nanometer to molecular scales, which are based on the unique mechanical and electromechanical properties of nanotubes, will be presented. Future directions and challenges for this field will be discussed.

2:00 PM A3.2
NEGATIVE DIFFERENTIAL RESISTANCE IN NANOTUBE DEVICES F. Légerard, J. Renouf, IBM Research Division, T.J. Watson Research Center, Yorktown Heights, NY.
We present results of quantum transport calculations of the device properties of degenerately doped nanotube p-n junctions and undoped metal-nanotube-metal junctions. We show that both of these devices exhibit negative differential resistance, with very high peak-to-valley current ratios even at room temperature. The undoped junctions rely on the quasi-one-dimensional geometry of nanotubes and have no analog in bulk devices.

2:15 PM A3.3
QUANTUM TRANSPORT THROUGH INTERMOLECULAR NANOJUNCTIONS: ALPER BULDUM, JIJIAN ZHAO, CALIN BUIN, JIE HAN AND JIANGPING LU, DEPT. OF PHYSICS AND ASTRONOMY, UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL, NC.

Quantum transport properties of intermolecular nanotube junctions are investigated. Intermolecular conductance is found to depend sensitively on atomic scale registry of contacts and nanotube chirality. Contact resistance can vary several orders of magnitude with atomic scale modifications of the intermolecular conductance approaches that perfect nanotubes. Novel phenomena such as negative differential resistance, resonance conductance, and nonlinear variation of resistance with contact area are found. These unusual properties may lead to novel device applications.

2:30 PM A3.4
DYNAMIC CONDUCTANCE OF CARBON NANOTUBES
C. BALANDIN,1,2 M. BANGMORNO NARDELLI,2,3 J. WANG,2,3 AND H. GAO.2,3
1Department of Physics, NC State University, Raleigh, NC;
2Department of Physics, The University of Hong Kong, Hong Kong, CHINA; 3McGill University, Montreal, PQ CANADA

The dynamic conductance of carbon nanotubes was investigated using a nonequilibrium Green's function formalism within the context of a tight-binding model. Specifically, the AC conductance through "finite" and finite-sized nanotubes will be discussed for tubes of different helicities, heterocycles and defects. Because of the induced displacement currents, the dynamic conductance of nanotubes differs significantly from the DC conductance displaying both capacitive and inductive responses. The present role of phonons assisted transport through nanotubes is revealed, and its implications for experiments discussed.

SESSION A4: ELECTRONIC PROPERTIES II
Chair: Ray H. Baughman
Monday Afternoon, November 27, 2000
Grand Ballroom (Sherraton)

3:15 PM A4.1
NMR STUDIES OF SINGLE WALLED CARBON NANOTUBES

In previous work we studied the electronic properties of single walled carbon nanotubes (SWNT) by nuclear magnetic resonance. 13C spin lattice relaxation times (T1) to determine the density of states at the Fermi Level. Since NMR measures the local density of states, different types of SWNTs with different local density of states can be resolved. Indeed, two types of SWNTs are observed. In some samples, one-third of SWNTs relaxes about 10 times faster than the other two-third of SWNTs. The fast-relaxing component is attributed to metallic SWNTs and the slow-relaxing component is attributed to semiconducting SWNTs. The spin-lattice relaxation rate of the fast-relaxing component is proportional to the temperature as expected for metallic systems. From the T1 data the density of states at the Fermi level can be estimated. The determined value agrees well with theoretical calculations. The electronic properties of SWNTs might change with exposure of the sample to molecules which adsorb on to the tubes or interfere with the bundles. The molecules can be introduced in gas form (H2, O2, O3, He, air) or through solid state reaction. We studied the effect of the adsorbed molecules on the relaxation behavior of the 13C spins and find significant decreases in T1 for Li, O2 and air. A smaller decrease in T1 was observed for He and no change was observed upon exposure to H2 and N2.

3:45 PM A4.2
ELECTRONIC STATES OF ALKALI METAL DOPED SINGLE WALL CARBON NANOTUBE AGGREGATES STUDIED BY LOW TEMPERATURE NMR.
Hironori Ogura, Kyu Yuki, Institute for Molecular Science, Okazaki, JAPAN, Syunji Bandow, ICORP-JST, JAPAN; Syojo Kuno, Yakushi Sato; Dept of Electrical and Electronic Engineering, Mie University, Tottori, JAPAN

Electronic states of alkali metal doped single wall carbon nanotube aggregates (SWNTs) below 100 K were studied by 13C-NMR. The state in this study was used in this study was used to evidence the DC arc discharge method using non-ferrimagnetic Pt-Re mixed catalyst. Amorphous carbon contained in the raw soots were removed by using hydrogen peroxide (H2O2). Doping of alkali metals were performed by so-called two-tube method. Recovery of 13C-labeling for undoped SWNT was found not to obey the single exponential law. This fact suggests the existence of two kinds of nuclear spin components below 100 K, i.e. fast-relasing spins which may be attributed to metallic tubes and slow-relasing spins to semiconducting tubes. On the other hand, we found that single exponential curve fitting can reproduce the data points of 13C-labeling for K-doped SWNTs sample. The value of 13C-T1 was found to become smaller by K-doping. Moreover, we found that the value of 13C-T1 become much smaller by using SWNTs samples after appropriate heat treatment as a starting sample.

4:00 PM A4.3
STM IMAGING OF CHIRAL METALLIC CARBON NANOTUBES.
A. Minimal, N. Wilson and C.L. Kane, DEPARTMENT OF PHYSICS, LABORATORY FOR RESEARCH ON THE STRUCTURE OF MATTER, PHILADELPHIA, PA.

Energy resolved STM imaging of short carbon nanotubes offers a unique opportunity for probing the wavefunction of the discrete electronic states. However, interpretation of such images will be complicated for two reasons. (1) Since the electronic states of the nanotube have two bands, the structure of the wavefunctions [and thus the image] is determined by the 2 by 2 reflection matrices characterizing each band. In all but non-chiral tubes with high symmetry gaps, reflection will mix the bands in a non-universal way. (2) Symmetry of the STM tip is known to severely modify the images of nanotubes and graphite: the STM image is not simply a picture of the wavefunction. We have developed a framework for calculating the STM tunneling density of states for chiral nanotubes, taking into account both the tube-ends and tip effects. By focusing on the longest wavelength Fourier components of the STM image we show that it is possible to "calibrate" the STM tip with three parameters. Since there are two bands there are two distinct classes of wavefunctions on the tubes. The images of the two wavefunctions contain enough information to determine the tip calibration, and the orthogonality between the two states leads to a nontrivial pair of constraints on the images. In this way, the wavefunctions of the eigenstates can be measured.

4:15 PM A4.4
WORK FUNCTION OF CARBON NANOTUBES.
Masanori Ando, SONY Corporation, Frontier Science Laboratories, Yokohama, JAPAN.

Carbon nanotubes (CNTs) is recognized as a fascinating material for nano scale electronic device (1) for the variety of electronic structure and one-dimensional geometry. The work function (W.F.) is one of the basic physical quantities to determine the electronic structure of the CNT metal interface and it is essential to know the precise value for device fabrication. There is a room for discussion on the value of W.F. of CNTs and there have been many reports by various methods. We studied the W.F. of CNTs by open-counter photoelectron emission spectroscopy (PES) system. While there is a difficulty in the measurement of vacuum-exposed materials by ultraviolet photoelectron spectroscopy (UPS), the PEE method makes it easy and precise work function measurements possible. We found that the W.F. of multi-walled CNTs is 4.95eV and that of single-walled CNTs is 5.05eV. For single-walled CNTs, this value is not significantly different from the previously reported value of 4.8eV as measured by UPS method (2). For comparison, we measured the W.F. of highly oriented pyrolytic graphite (HOPG) which is considered as an orthogonal \pi-\sigma valence state. The measured value was 4.85eV, slightly smaller than that of CNTs. Because CNTS has a non-orthogonal \pi-\sigma valence state, the experimental results can be interpreted as a rotation of different valence states between HOPG and CNTs. First principle ab-initio calculation was carried out and the experimental data were well reproduced in this calculation.

References:
(2) S. Suzuki et. al., submitted in Appl. Phys. Lett.

4:50 PM A4.5
EFFECT OF TRANSITION METAL IMPURITY ON TRANSPORT PROPERTIES OF SWNTS.

Electrical transport properties in as-synthesized SWNTs are now...
known to be sensitive to oxygen doping under ambient conditions [1, 2]. Degasifying samples in vacuum at 500 K drives the thermopower negatively, indicating that dissolved metallic tin is not the origin of the monolaminate large value of thermopower is still not clear. Recently, the coupling of the conduction electrons in SWNTs with localized magnetic moments of residual transition metal catalysis impurity (Kondo effect) has been shown to dominate properties of these nanomolecules [3]. We present results of thermopower and resistivity as a function of residual catalyst concentration (as determined by TGA analysis) through a series of purification steps which successively remove the Ni impurity in the samples. We have found the suppression of the Kondo peak in the thermopower of O$_2$ doped and degassed SWNTs correlates with the amount of Ni in the samples. Temperature dependence of the resistivity shows almost no change with the amount of Ni suggesting low temperature upturn in resistivity has different origin other than the Kondo effect. This work was supported by Grants NSF DMR 98-09686 and DOD DAAD19-97-C-3885 [1]. P. M. Collins, et al., Science, 287, 622 (2000) [2] G. U. Jumape, et al., accepted for Phys. Rev. Lett. 85 (1999) [3] G. Grigoriu, et al., Phys. Rev. B 60, 113109 (1999)

4:45 PM A4.6
POLARIZED-ROTATIONAL ELECTRON TRANSPORT IN CARBON NANOFLATERS, Dirk Organski, Gary J. Mankey, Hide Fujiwara, Univ of Alabama, MINT Center, Tuscaloosa, AL.

Electronic transport measurements in multilayer carbon nanotubes indicate the possibility for ballistic (Blank et al., Science 280, 1744) and spin-coherent (Tanaka et al., Nature 401, 572) electron transport. We present spin-polarized transport measurements on carbon nanotubes contacted by ferromagnetic electrodes. The electrodes are prepared by electron-beam evaporation through a shadow mask. In contrast to previous measurements the gap between the electrodes is as wide as a micrometer. The observed magnetic-resistance effect is consistent with a mean free path for spin-flip scattering of at least 400 nm.

SESSION A5: PROCESSING AND PURIFICATION
Chair: Zhifeng Ren
Tuesday Morning, November 28, 2000
Grand Ballroom (Saratoga)

8:30 AM A5.1
MAGNETICALLY ALIGNED MEMBRANES OF SINGLE-WALL CARBON NANOFLATERS, D.A. Walters, Univ of Central Florida, Dept of Physics, Orlando, FL; M.J. Cozzarelli, X.C. Qin, J.J. Schmidt, C.B. Huffman, K. Smith, D.T. Colbert, R.E. Smalley, Rice Univ, Ctr for Nanoscale Science and Technology, Houston, TX.

Nanotubes have exceptionally anisotropic properties: mechanical, optical, thermal, electronic, and magnetic. In order to measure and apply these properties, we prepared an aligned bulk solid of single-wall carbon nanotubes. Nanotubes were sonicated to produce a stable colloidal suspension containing mostly individual nanotubes and then deposited on top of a magnetic field. A magnetic field was applied to align a magnetic field; the average alignment energy was 28 times thermal energy at room temperature. Under similar conditions, a nanotube was filtered in the presence of a magnetic field and the alignment was preserved. An aligned membrane of nanotubes. The magnetically aligned membrane displays anisotropic mechanical, optical, thermal, and electronic properties. Its density is over half of the theoretical bulk density of close-packed nanotubes. Such a well-defined, highly aligned membrane of nanotubes. The magnetically aligned membrane displays anisotropic mechanical, optical, thermal, and electronic properties. Its density is over half of the theoretical bulk density of close-packed nanotubes. Such a membrane is a valuable model system for studying nanotube properties. The latest results of which will be discussed.

9:00 AM A5.2
SIMPLE AND COMPLETE PURIFICATION OF SINGLE-WALL CARBON NANOFLATERS, A.C. Dillon, J.L. Allamane, K.M. Jones, P.A. Parsons, M.G. Heben, National Renewable Energy Laboratory, Golden, CO; T. Gennett, Department of Chemistry and Center for Materials Science, Rochester Institute of Technology, Rochester, NY.

Carbon single-wall nanotubes (SWNTs) have a variety of unique physical, electronic, and mechanical properties. However, the SWNTs must be thoroughly purified if they are to be used in a variety of potential applications and basic studies. We employ a laser technique to that of an additional purification of SWNTs. When a single SWNT is exposed to the laser it produces a CO$_2$ emission and a significant rise in temperature. When this emission is observed, we conclude that the SWNT is a single nanotube.
found to have occurred and single-walled carbon nanotubes could no longer be observed. The graphitized structure contains a lot of cage-like structures, indicating that the single-walled carbon nanotubes can be regarded as non-graphitizing carbon.

SESSION 6: SYNTHESIS AND CHARACTERIZATION
Chair: Michael J. Heben
Tuesday Morning, November 28, 2000
Grand Ballroom (Sheraton)

10:30 AM A6.1

Following our success of aligned growth of large arrays of multiwall carbon nanotubes, we have extended this technique to grow carbon nanotubes on a variety of useful substrates such as tungsten coil, conventional STM tip, quartz fiber, etc. for applications such as lamp element, high resolution STM tip, scanning tunneling microscope tip, etc., respectively. SEM and TEM are used to examine the microstructure. In addition, we also discovered a new technique that can yield kilograms of multiwall carbon nanotubes at extremely low cost. Using the carbon nanotubes produced by this new technique, we have improved conductivity by 250 times in the electrophilic polymer film.

We have also succeeded to synthesize electrodes with capacity above 200 F/g which is very much desired for Li battery applications and energy storage.

10:45 AM A6.2
WELL-ALIGNED CARBON NANOTUBES SYNTHESIZED BY ELECTRON CYCLOTRON RESONANCE CHEMICAL VAPOR DEPOSITION. F. Hashi, T. Tahakura, FCT Research Dept., Japan Fine Ceramics Center, Tsukuba, JAPAN; S. Yamashiki, Frontier Technology Research Institute, Tokyo Gas Co., Ltd, Yokohama, JAPAN; K. Taniyama, A. Moto, FCT Research Dept., Japan Fine Ceramics Center, Tsukuba, JAPAN; M. Yamamota, National Institute of Materials Research, Tsukuba, JAPAN; T. Hirao, Osaka University, Osaka, JAPAN; S. Fujimori, Y. Koga, National Institute of Materials Research, Tsukuba, JAPAN.

Well-aligned high density carbon nanotubes (CNTs) perpendicular to metal thin films deposited on n-type Si (100) substrate have been synthesized successfully by electron cyclotron resonance plasma enhanced chemical vapor deposition (ECR-CVD). The metal thin films were coated on the substrate using vacuum evaporation method. The metal of Ni, Fe, Co, and Ni was utilized. CNTs were grown at 550-800°C. Methane is used as the carbon source for the growth of the CNTs with the mixture of hydrogen and argon. The applied microwave power and the pressure during the growth of CNTs were 800 W and 1.8 x 10^-3 Pa, respectively. The growth time of the CNTs was maintained for 30 min. The morphology of the CNTs was examined by scanning electron microscopy. The CNTs with diameter in the range of 50-80 nm were obtained in this study. The length and the density of CNTs range from 1.5 to 2 µm and from 10^8 to 10^9 cm^-2, respectively. Transmission electron microscopy images reveal the CNTs to be multiwalled tubes. We examined the diameter and uniformity of the CNTs as a parameter with plasma intensity and methane, hydrogen and argon gas ratio, and their flow rates. The ECR-CVD process has characteristics of high plasma density at low temperature, less ion damage, contamination-free and high deposition rate. Thus the ECR-CVD process is a suitable method to synthesize the CNTs of large area. Moreover their electron field emission characteristics have been measured, showing that high density, devices requiring freestanding vertical CNTs such as scanning probe microscopy, field emission flat panel displays, etc. can be fabricated without difficulty.

11:00 AM A6.3
UNUSUAL RESONANCE RAMAN SCATTERING FROM HIPCO-DERIVED SWNTS. A.A. Sienko, P.C. Ekwall, Dept. of Physics, Pennsylvania State University, University Park, PA; M.J. Bronikowski and R.E. Smalley, Rice University.

We have carried out resonant Raman scattering studies of nanotubes obtained from different batches of SWNT material made at Rice University by catalytic growth in higher pressures of CO with Ni-catalyst (HIPCO). The Raman spectra using visible excitation is similar to the other bundles of SWNTs produced by the arc discharge and pulsed laser vaporization methods. That is, the spectra exhibit the characteristic radial breathing and tangential Cntam displacement modes. However, the resonance curve, i.e., Raman cross section vs. laser excitation energy is strongly sensitive to the HIPCO synthesis conditions, with the maximum in the cross section shifting by about ∼0.5 eV from one HIPCO sample to the other. Careful electron microscopy and transport measurements suggest that these HIPCO nanotubes can be regarded as non-graphitizing carbon.

11:15 AM A6.4

Carbon single-wall nanotubes are routinely produced by various methods and they are most often collected as two-dimensional microcrystals of tens of individuals. In order to investigate the effect of intertube interactions on vibrational properties of these ropes, we use a pair potential approach for the evaluation of van der Waals binding. In a continuum limit, we show that the intertubes-rod radius range from 5 cm to 60 cm [1], depending on the number of tubes in the bundle and on the tube diameters. We also present dispersion curves of infinite arrays of nanotubes and have found that the sound velocity are 1226 m/s and 806 m/s for the two acoustic phonon branches [2]. On another hand, we focus on the so-called radial breathing mode (RBM). Indeed, this low frequency fully symmetric Raman active mode is one of the more popular nanotube signature for the characterization of samples. From both rigid cylinder approach [1] and valence force field [3], we have found that the van der Waals interaction upshifts the resonant frequency by 10% for 10 infinite bundles and that this value is already reached for a bundle of 20 tubes. For smaller bundles, the more intense breathing mode appears at intermediate frequency and a complex excitation scheme that depends on the symmetry of the bundle. Moreover, from a Valence Force Field calculation, we found that the tubes [larger than (10,10) bundles], can hardly be considered as rigid breathing cylinders and that the smaller upshift and the splitting of modes that are observed in this case can be explain by this softening. We also investigate the RBM signature of the bundles is found to be different from the superposition of individual nanotube excitations. [1] L. Herrard, E. Hernandez, P. Bernier, A. Rubio, Phys. Rev. B 60 (1999) R5291 [2] L. Herrard, Ph. Lambin, A. Rubio. Proceedings of the IWEPM 2000, Kirchberg, In Press [3] V.N. Popov, V.E. Van Doren, M. Balkanski. Phys. Rev. B 59 (1998) R5355

11:30 AM A6.5
POLARIZED RAMAN SPECTRA OF CARBON NANOTUBES. Ado Jorio, Sandra D.M. Brown, Gene Dresselhaus, Milled S. Dresselhaus, Massachusetts Institute of Technology, Cambridge, MA; M.J. Pimenta, Universidade Federal de Minas Gerais, Belo Horizonte, BRAZIL; Rául Sato, Dept. of Electronics-Engineering, Univ. of Electro-Communications, Tokyo, JAPAN; Apparao M. Rao, Center for Applied Energy Research, Dept of Physics and Astronomy, Univ of Kentucky, Lexington, KY; Karin Kowarz, Dept. of Physics, Technical University of Berlin, Berlin, GERMANY.

We performed polarized resonant Raman spectroscopy (RRS) of single wall nanotube (SWNT) samples with different diameter distributions. Resonant Raman spectra from metallic or semiconducting SWNTs were selected by using different incident laser excitations. We discuss the dependence of the GBand on polarization geometry for the different nanotube samples, focusing on the polarized Raman spectra of metallic SWNTs, where the depolarization effect is strong. We compare the results with polarization Raman studies on semiconducting SWNTs and multiwalled carbon nanotubes. We also performed polarized surface-enhanced Raman studies (SERS) on SWNTs, and we compare the polarized SERS and RRS results.

11:45 AM A6.6
TEM STUDIES ON MULTIWALL CARBON NANOTUBES GROWN BY CHEMICAL VAPOR DEPOSITION. Jiawen Wen, Zhongping Huang, Wenjun Li, Yi Tu, Dezhi Wang, Jinhua Chen, Xiaoyang Yang, Zhifeng Ren, Department of Physics, Boston College, Chestnut Hill, MA.

An array of single freestanding multiwall carbon nanotubes (MWNTs) grown on a micrometer sized Si substrate by plasma enhanced chemical vapor deposition (CVD) are characterized by cross-sectional TEM to understand the microstructures of the tip, middle part, and the interface between substrate and nanotube. All single freestanding MWNTs we have imaged are hollow and capped by a graphite dome with a diameter of the curvature of about 2 nm. At such tip, one can always find an encapsulated single crystalline Ni cylinder. Micro-
structures at interface show that the outer diameter of multivall carbon nanotubes is determined by the size of the nanodisk. The growth mechanism at interface of the growth will be discussed based on these microstructures. Our characterization indicates that arrays of freestanding MWNTs with sharp tip (2 nm radius), controlled diameter, length, and site spacing (1 and 2 micrometer) have been achieved by photolithography, patterned CVD. Structure of MWNTs grown on silicon and graphite foil by CVD have also been studied by high-resolution TEM (HRTEM) and image analysis. With this technique, we found that the chirality of MWNTs can be determined quickly by the HRTEM image and diffraction pattern. Zigzag, armchair of armchair and zigzag, and other chiral MWNTs have been observed. Furthermore, we found that many of the three 100[1] latice fringes in the center of nanotube is used to determine the chirality of a MWNT, which is of great importance to rapidly establishing the relationship among the properties, structure, and growth conditions of carbon nanotubes. The broken microstructures of MWNTs with different chiralities under tensile strength will also be presented.

SESSION A7: MECHANICAL PROPERTIES
Chair: Tamir Yildiz
Tuesday Afternoon, November 28, 2000
Grand Ballroom (Sheraton)

1:30 PM A7.1
NANOTUBE MECHANICS. Min-Rong Yu, Oleg Lourie, Richard Piner, Henry Rohrs, Kevin Aslam, Hui Huang, Rodney S. Ruoff, Dept of Physics, Washington University, St. Louis, MO.

We have designed, built, and used new tools that operate inside of electron microscopes (SEM) and separately, TEM to pick up, attach, and mechanically load nanotubes. Stress and strain are determined from direct EM imaging of the operating nanomechanical stages. Results from such experiments will be presented.

2:00 PM A7.2

The concept of a continuum elastic shell provides a useful reduced description for quasi-two-dimensional objects, as soon as their parameters are well determined. We have computed the in-plane stiffness, flexural rigidity, shear modulus and Poisson ratio for the mononatomic layers and tubules of carbon, boron nitride and the novel forms of fluorinated carbon. Using the same gradient corrected PBE density functional together with the periodic boundary conditions [1] has allowed to test the limits of linear elasticity and to consistently compare the properties of these materials. A noticeable equilibrium curvature of the C2F has been predicted, in contrast to the nearly flat BN and C sheets. We further apply these parameters to estimate the elastic energy of lateral compressibility, and the bending (compressive) strength of multivall nanotubes [2], where the interplane van der Waals forces begin to play significant role.


2:15 PM A7.3
MECHANICAL PROPERTIES OF CHARGED CARBON NANOTUBE. Jianwei Che, Xin Xu, Takis Cagin, and William A. Goddard III, Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA.

Over the past decade, both theory and experiment have shown that carbon nanotubes have both unique electronic properties (e.g. it may be semiconducting or metallic depending on the chirality) and extreme mechanical strength (e.g. tensile modulus >1 TPa). Consequently, there is considerable interest in designing and manufacturing functional devices and novel composite materials based on carbon nanotubes. In particular, we have considered how introducing and controlling charges in various locations might modify the mechanical properties of carbon nanotubes. In agreement with experiments by Baughman et. al [3], we find that introducing excess charges into nanotubes can lead to mechanical deformations that do not coincide with the deformations seen between tube deformation and stress and the charge distribution using tight-binding electronic structure theory. In addition, we have determined how the vibrational modes are affected by charge injection and the implications for the stability of carbon nanotubes. These results suggest a wide range of practical implications, including the design of nano-electro-mechanical systems (NEMS) and nano-actuators. Reference: 1. R.H. Baughman, C. Cui, A.A. Zakhidov, et. al., Science, 284, 1343 (1999).
bond rotations. Molecular dynamics allows to generate an atomic configuration of the junction [20,19],[20,20],[20,19] which matches well the observations, the "force field", and the resulting electronic property sequence observed in the experiment. It provides first evidence of the effect of mechanical modification on the local electronic structure of CNT.

**3:45 PM A8.2**

**MANUFACTURE AND CHEMICAL MODIFICATION OF INDIVIDUAL CARBON NANOTUBES AS PROBES FOR TOPOGRAPHICAL AND CHEMICAL SENSORS.** Ninni Clici, Tatsuki Uchihashi, Tetsuo Shimizu, Susanne P. Jarvis, Wataru Minami, Hiroshi Takemoto, JRCAT, Tsukuba, Ibaraki, Japan; Seji Akiti, Yoshikazu Fujisawa, Osaka Prefecture University, Suita, Osaka, Japan; Atsushi Ando, Electrotechnical Laboratory, Tsukuba, Ibaraki, Japan.

Carbon Nanotubes (CNTs) are of great interest from the viewpoint of their unique electronic and mechanical properties, chemical stability, and potential application in molecular devices as well as probe tips for atomic force microscopy (AFM). To prepare CNT-tips, two techniques have previously been demonstrated. One is to attach CNT onto a commercial tip either by using adhesive carbon tape under an optical microscope or by depositing amorphous carbon in a scanning electron microscope (SEM). The second is to grow a CNT at the apex of the tip by a chemical vapour deposition technique. With these techniques, it can be difficult to control important parameters such as the length of CNT tip (except for shortening by cutting which produces an open end), the direction of the CNT tip, and the formation of good mechanical and electrical interfaces between CNT and tip. To overcome these problems, we have developed a new manipulation system as an assembly technique. This consists of two sets of piezoelectric stages with which we can adjust accurately both the position and orientation of the CNT tip. In this talk, we will explain how this system manipulates CNT and shows several AFM applications.

**4:00 PM A8.3**

**THE FABRICATION OF CARBON NANOTUBES FOR NANO-DEVICES AND BIOSENSORS.** Jun Li1, Hossin Ng1, Jianmin Fu2, Angang Pang2, Roderick Y.H. Lim1, Weide Zheng1, Yinfeng Xing2, Guoqin Xu1, Stephan Jeswiet2 and Sun F.Y. Li1,1. Institute of Materials Research & Engineering, SINGAPORE, National University of Singapore, Dept of Chemistry, SINGAPORE.

Carbon nanotubes (CNTs) have shown delicate macromolecular structure and extraordinary materials properties. This class of materials has provided great application potential in the upcoming nanotecnology [21] and we report on our findings in three issues: [1] mass production, [2] direct growth of CNTs into nanodevices, and [3] application of CNTs in chemical and biological sensors. Recently, chemical vapor deposition (CVD) has been recognized as an attractive method due to many advantages; the selection of catalysts and the control of the size of catalyst particles have been known to play an important role. We have developed a method to synthesize CNTs by CVD using catalysts impregnated in a monospecific support. This monospecific catalyst support has an ordered hexagonal array of uniform, one-dimensional channels with pore sizes tunable from about 2 nm to 30 nm, which is exactly in the range of the outer diameters of carbon nanotubes and it can be impregnated with any metal. Arrays of carbon nanotubes can be controlled by this substrate.

Many applications of carbon nanotubes rely on the ability to control the growth of carbon nanotubes into regular microarrays or deliberately scaffolded structures. Here, we demonstrate a non-contact lithographic approach to pattern solution-based organometallic precursors onto novel flexible substrates. Highly ordered and uniform arrays of CNTs could be directly grown on these templates by CVD methods with controlled alignment and configuration, which may be useful for future device fabrication such as field emission displays and sensors. By making use of the physical shrinking properties of polyethylene terephthalate at high temperatures, we extended this approach to the fabrication of a networked complex network of CNT membranes. We will show that this membrane can be used in electrochemical sensors and gas sensors.

**4:15 PM A8.4**

**PROPERTIES OF CARBON NANOTUBE PROBES FOR ATOMIC FORCE MICROSCOPY.** Katerina Mokoni, Max Logally, PIEZOMAX Technologies, Milton, WI.

We have investigated a number of properties of multiwall C nanotube tips used as probes for atomic force microscopy (AFM). We mounted multiwall nanotubes bundles on conventional cantilever tips and amplified their ends. The advantages of C nanotubes for surface profiling are, of course, the high aspect ratio and the compliance of the probe. So that high resolution is not sacrificed for the sake of high aspect ratio, the bundles are sharpened using a method we developed. We have profiled a variety of high-aspect ratio nanotubes in Si, including 280nm wide and 650 nm deep trenches as well as 2:3 micron deep features. We demonstrate that our tips are capable of imaging deep and narrow trenches (side wall angles of 88 degrees). We have made comparative studies of tip-sample interactions with C nanotube probes and conventional Si or Si nitride AFM tips to determine the lifetime of the tips and simple degradation with both hard and soft samples. Whereas conventional tips cause significant sample damage, C nanotube tips do not. Similarly, conventional tips wear rapidly, losing resolution, whereas C nanotube probes maintain their resolution and thus have a minimum usable lifetime at least an order of magnitude greater than conventional tips. We will also present preliminary but very positive results using C nanotubes coated with magnetic material for obtaining magnetic force microscopy (MFM) images. Finally, we show a variety of C nanotube AFM imaging applications in a wide range of materials. Supported by DARPA SBIR program. [1] patent applied for.

**4:30 PM A8.5**

**IN-SITU SINGLE-WALLED NANOTUBE TIPS FOR ATOMIC FORCE MICROSCOPY.** Jason H. Hafer, Chin-Li Cheung, Charles M. Lieber, Harvard University, Dept of Chemistry and Chemical Biology, Cambridge, MA.

The unique properties of carbon nanotubes make them ideal atomic force microscopy (AFM) probe tips. Previously, the fabrication of carbon nanotube tips was limited to laborious assembly or catalytic tip preparation procedures and only produced multi-walled nanotube bundles or single-walled nanotubes, which limited the imaging resolution. A new chemical vapor deposition based synthesis approach will be described which allows simple and reproducible fabrication of individual multi-walled nanotube tips with ca. 1 nm radii, yet are mechanically rigid due to the high Young’s modulus of carbon nanotubes. Images of spherical gold nanoparticles on mica demonstrate the expected high resolution based on the nanotube tip structure. Force spectroscopy and high resolution imaging with nanotube tips demonstrates that they elastically buckle rather than fracture under large loads, making them highly robust probes. The nanotube tip length is critical as it strongly affects the buckling force, lateral stiffness, and thermal vibration amplitude of the tip. An etching technique will be described which allows control over the nanotube tip length with 2-nanometer precision. The unique combination of high resolution and high aspect ratio of the nanotube tips allows structural state of large, isolated proteins to be imaged by other methods. Recent results in this area will be presented.

**4:45 PM A8.6**

**USE OF MULTI-WALLED CARBON NANOTUBES FOR CONDUCTIVE PROBE SCANNING FORCE MICROSCOPY (CP-SFM).** Kevin B. Stevens, Ronald P. Andres, Purdue Univ, Dept of Chemical Engineering, W. Lafayette, IN.

Multi-Walled Carbon Nanotubes (MWNs) mounted on commercial SFM cantilevers have proven to be excellent probes for high resolution Tapping Mode Scanning Force Microscopy [TM-SFM][1]. Because of their robust nature and relatively high electrical conductance, MWNs are also attractive for use in Conductive Probe Scanning Force Microscopy [CP-SFM]. To be used in this application, however, the MWN must be mounted via a high conductance contact to a conductive cantilever. The technique employs a spatially selective electro-deposition of gold to mechanically and electrically secure a MWN to the tip of a gold plated silicon cantilever. The thin gold adhesion provides good electrical contact between the cantilever and the MWN allowing the MWN to be used as a conductive probe. Preliminary measurements indicate this probe behaves in anionic manner. The superior mechanical adhesion provided by this technique also produces an extremely robust probe for both TM-SFM and CP-SFM studies. [1] Mekoni K, Bass M.R., Andres R.P., ULTRAMICROSCOPY 80(4):237-246 DEC 1999

**SESSION A9: HYDROGEN STORAGE IN CARBON NANOTUBES**

Chair: John E. Fischer
Wednesday Morning, November 29, 2000
Grand Ballroom (Sheraton)
NOTE EARLY START

8:15 AM #A0.1
RAPID, ROOM TEMPERATURE, ATMOSPHERIC PRESSURE STORAGE OF HYDROGEN IN SWNTS. Michael J. Heben, Anne C. Dillon, Jeffrey L. Allen, Kim M. Jones, and Philip A. Parilla, National Renewable Energy Laboratory, Golden, CO, Thomaas Gennett, on sabbatical from Department of Chemistry and Center for Materials Science, Rochester Institute of Technology, Rochester, NY.

As we demonstrated in 1997 [1], single walled carbon nanotubes are capable of adsorbing hydrogen at room temperatures and pressures. Early experiments were performed on highly impure samples. Although hydrogen storage densities were estimated to be between 5 and 10 wt% on a SWNT weight basis, the amount of hydrogen stored on the total sample was only ~0.1 wt%. Since that time we have developed methods for obtaining SWNTs in purities as high as 98 wt% [2], and also developed methods to activate these materials for hydrogen storage. Hydrogen can be stored on these materials at 6-7 wt%. The activated SWNT material can be charged in a matter of minutes at room temperature and normal atmospheric pressure.

Temperature programmed desorption spectroscopy shows that there are two distinct sites for hydrogen adsorption. Approximately 2/5-3/5 of the total hydrogen is in a low temperature site that can easily be removed at room temperature. The remaining 3/5 of the hydrogen is more stable and is not removed until temperatures greater than 300°C. Since the hydrogen-charged samples are fairly stable in air they can be investigated with a variety of ex situ techniques. In particular, Raman spectroscopy has been used to observe that charge transfer from the hydrogen to the carbon nanotubes occurs intact. We will discuss these results in detail with particular attention to the relationship between electronic and structural factors.


8.45 AM #A0.2
CARBON HYDROGEN STORAGE IN CARBON NANOTUBE-BASED MATERIALS. Ping Chen, Jinjy Li, Kung Lee Tan, Dept. of Physics, National University of Singapore, Singapore, SINGAPORE.

Much attention has been paid to the hydrogen storage by carbon nanotubes. Unlike single-wall carbon nanotubes, the multi-wall carbon nanotubes absorbs substantial hydrogen only after being treated with alkali metals. Recent experiments have shown that hydrogen is adsorbed into the multi-wall carbon nanotubes and confirm the amount of hydrogen uptake by the material. It was found that the conditions in preparation and pre-treatment of alkali metal-doped carbon nanotubes strongly affected the capability of hydrogen storage. Characteristic studies show that a new phase of alkali and carbon is formed, and the tubular structure is somewhat destroyed. The electronic and structural changes in carbon nanotubes will favor the chemical absorption of hydrogen. The behaviour of contaminants, such as moisture and oxygen, in the hydrogen absorption process was also investigated.

9.15 AM #A0.3
HYDROGEN DESORPTION MEASUREMENTS ON CARBON NANOSTRUCTURES. Michael Hirschcr, Marion Becher, Ursula Delaff-Weglkowska, Max-Planck-Institut für Metallforschung, Stuttgart, GERMANY; Andrea Quintel, Verra Schalkow, Young-Mo Choe, Miro Halkoš, Segnar Roth, Max-Planck-Institut für Festkörperforschung, Stuttgart, GERMANY; Ingrid Stepanek, Patrick Bernier, University of Montpellier II, Montpellier, FRANCE.

Measurements of the hydrogen storage on single-walled carbon nanotubes (SWNTs) and graphite will be presented. SWNTs have been purified, opened and surface cleaned by various methods, such as boiling in different acids, oxidation, ultrasonication, mechanical grinding, and ball milling. The specimens have been well characterized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, and Raman spectroscopy. The hydrogen content is investigated by thermal desorption spectroscopy utilizing a mass spectrometer. The effects of the different treatments on the hydrogen storage capacity will be discussed. These investigations indicate that an opening of the SWNTs is essential to reach high storage capacities. We thank the DffG for financial support.

SESSION A10: HYDROGEN STORAGE AND INTERCALATION

Chair: Peter C. Ekund
Wednesday Morning, November 29, 2000
Grand Ballroom (Sheraton)

10:15 AM #A10.1
DEEP INELASTIC NEUTRON SCATTERING STUDIES OF H2 IN CARBON NANOTUBES. David Narechko, Paul Skol, Peter Eklund, Dept. of Physics, The Pennsylvania State University, University Park.

Deep Inelastic Neutron Scattering (DIS) provides a unique microscopic perspective of the state of adsorbed molecules on nanotubes. We report DIS studies of H2, H2O, and adsorbed on bundles of SWNTs at 15K. We find that the J = 1 → J = 0 conversion rate for the adsorbed molecules is anomalously high. This rate is too fast to measure in our studies. We can, however, place a lower limit on the rate of 1000s of an hour. This enhancement of 1000 over the rate in liquid H2 DIS studies yielded spectra consisting of multiple peaks, due to rotational transitions, with widths determined by the translational momentum distribution n(R).

The mean kinetic energies obtained from the width of the n(R) is 1.04±0.05 eV, slightly lower than observed on planar graphite surfaces. These values are much lower than theoretical predictions for H2 adsorbed in the interstices between tubes, indicating that H2 does not adsorb either on the outer surface of the bundles or in the core of the tubes. The measured rotational energy levels are 4-5 times those of bulk H2. However, the rotational form factors associated with the transitions are much different than the bulk values indicating a significant modification of the rotational wave function of the molecule. The modification of the rotational wave function, which is not observed for H2 on planar graphite, may indicate the primary adsorption sites are in the core of the tube. This work was supported by the NSF DMR 9707026 (MERSEC) and Honda.

10:30 AM #A10.2
ADSORPTION AND QUANTUM ROTATION OF HYDROGEN IN SINGLE-WALL CARBON NANOTUBES. C.M. Bera, V. Tiwari, T. Yikiririm5, D.A. Neumann5, J.E. Fischer5, M.J. Heben5.
5University of Maryland, College Park, MD, 6National Institute of Standards and Technology, Gaithersburg, MD, 7Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, 8Center for Basic Science, National Renewable Energy Laboratory, Golden, CO.

Adsorption of atoms or molecules in nanopores may have considerable fundamental interest because of two main reasons: the reduced dimensionality and technological importance, such as gas separation and hydrogen storage. We report hydrogen adsorption isotherms in single-wall carbon nanotubes as a function of pressure, temperature, and various sample treatments. The loading isotherms are compared with various model calculations based on Monte Carlo simulation in the grand canonical ensemble. Neutron scattering techniques are used to characterize the SWNT samples and to probe the dynamics of hydrogen molecules trapped in nanotubes. The inelastic neutron scattering measurements clearly show the ortho to para conversion of physically adsorbed hydrogen in nanotubes containing small amounts of hydrogen. Unlike H2 adsorbed in solid C60, the conversion dynamics is fast, which is attributed to the paramagnetic metal impurities in the sample. From the rotational J = 0 → 1 transition, no indication of a significant barrier to quantum rotation seems to exist. The dynamics of the temperature dependence of the J = 0 → 1 transition was investigated and compared to those observed in graphite and solid C60.

10:45 AM #A10.3
DOPING PROPERTIES OF POTASSIUM INTO SINGLE WALL CARBON NANOTUBES BY VAPOR PHASE REACTION. Shanjing Baozong, Miko Tokunzawa, Japan Science and Technology Corporation, Dept. Materials Science and Technology, Meijo University, Nagoya, JAPAN; Sumio Iijima, Japan Science and Technology Corporation, NEC Corporation Tsukuba and Meijo University, Nagoya, JAPAN.

The doping of K to the interstitial site of (10,10) single-wall carbon nanotube (SWNT) bundles is a candidate for the superconductor [1: S. Sato, MRS 1999 Fall Meeting Proceedings]. The stoichiometry of the material is KxC60 [x]. In order to increase the density of K in the interstitial site at the Fermi level, the doping into the interior site of SWNT is more favorable. When the K is fully doped to both the interior and interstitial sites of SWNT bundle, the stoichiometry will be represented by K9C60. Recently, we have found a method for doping the various fullerenes into the interior site of SWNT with high yield (poster presentation by K. Hirahara et al). The samples in the present study were synthesized by using this technique and prepared two types of K-doped SWNTs, one considered to correspond with K6C60 (interstitial doped SWNTs) and the other is K9C60 (interior doped SWNTs) and K12C60 for interior and interstitial doped SWNTs. However, the stoichiometric ratios have not yet been confirmed by experiment. Therefore, in the present study, we measured the electrical resistance of the K-doped SWNTs by electrical conductance (ESR) and Raman scattering. From these results, we found that the value of the Pauli paramagnetic slope was increasing with K6C60 sample indicated smaller value by ~1/3 (average) than that for
alkali-doped samples were evidenced by drastic changes in the resonant Raman spectra [1]. Here, we probe the mechanisms of alkali intercalation and charge transfer by in situ Raman investigations coupled with conductivity measurements performed during a gas-phase doping experiment. We measure different characteristic spectra which we assign to different stoichiometries and degrees of charge transfers [2]. Our conclusions are supported by further Raman investigations on Li-doped SWNT samples. The Li-doped SWNTs are prepared via redox reactions between SWNT and solutions of organic radical-anions, using Li as a counter ion which allows to control the charge carrier concentration in the nanotubes [3]. Different Raman responses are measured and associated to different level of doping. [1] A.M. Rao et al, Nature 388, 257 (1997). [2] N. Ben-dor et al, to be published. [3] E. Jouguet, C. Mathis and P. Petit, Chem. Phys. Lett. 318, 561 (2000).

SESSION A11: CHEMICAL MODIFICATION
Chair: Anne C. Dillon
Wednesday, Afternoon, November 29, 2000
Grand Ballroom (Sheraton)

1:30 PM A11.1
FIXATION AND ORGANIZATION OF PROTEINS AROUND CARBON NANOCTUBES. F. Balkowie, C. Richerd, P. Schuz, C. Moskowitz, CEA Saclay and U. Stranburg, Gif sur Yvette, FRANCE.

Carbon nanotubes have been used as supports for the fixation and crystallization of proteins. The linkage between the nanotubes and the proteins was realized via bi-functional linkers which have two different binding sites to the tube surface. This approach make possible the assembly of a given protein or protein complex with defined orientation and distance. The translation of the proteins around the nanotubes has been observed. Applications toward the development of nano-biosensor are under way.

2:00 PM A11.2

Dynamical properties of the SWNTs were investigated using solid state NMR on purified SWNTs. The temperature dependence study reveals a maximum at 170K in the relaxation rate that we attribute to molecular dynamics of small amplitude of the tubes inside the ropes. The obtained results are in agreement with previous findings from neutron experiments. An important question arises concerning the modification of the electronic properties by the purification procedure. On the functionalised SWNTs using cross polarization and decoupling NMR techniques we identify the chemical modifications induced by the purification treatment, in particular carbolic groups could be observed. These functional groups on the tube surface can be regarded as defects which may modify the SWNTs' properties. NMR and ESR investigations providing evidence for such modifications will be presented.

2:30 PM A11.3
COMPARATIVE ADSORPTION OF SIMPLE MOLECULES ON SINGLE WALL CARBON NANOCTUBES. M. Benfai, K. Murr, J.P. Palmari, CRMC2-CNRS, Marseille, FRANCE; N. Dupont-Paolovsky, Laboratoire Chimie du Solide Matériel, Vandoeuvre-lès-Nancy, FRANCE; P. Zeppenfeld, Johannes-Kepler University, Linz, AUSTRIA; N. Dufau, Y. Grillet, CTM-CNRS, Marseille, FRANCE; B. Amsuss, University, Kiel, GERMANY; M. Johnson, ILL, Grenoble, FRANCE.

Methane, krypton, xenon and SF6 adsorption on single wall carbon nanotubes (SWCN) associated in bundles produced by the Montpellier group has been studied by adsorption isotherms measurements, calorimetry, quartz-elastic neutron scattering and neutron diffraction. Methane, krypton and xenon adsorption isotherms exhibit two steps corresponding to the adsorption on two types of compararibly uniform patches during the first stages of the adsorbate condensation. The values of the methane isosteric heat of adsorption on these two adsorption sites have been determined. They are in very good agreement with those measured by means of isothermal micro-calorimetry. In contrast with methane, krypton and xenon
xenon, SF6 adsorption isotherms exhibit only one step corresponding to the less attractive adsorption sites. These results are consistent with the adsorption data, for the first step, inside the interstitial channels between the nanotubes forming a bundle, except for the biggest molecule SF6 which cannot penetrate them, - for the second step, on the external surface of the bundles. The quasi-basics neutron scattering experiment was performed on CHI adsorbed on the same SWCNs in order to characterize the diffusivity of these molecules. It was shown that the sites of adsorption, previously observed by adsorption volumetry and calorimetry measurements, correspond to a solid-like phase for the more strongly bound site at T < 120 K and to a viscous liquid-like component for the more weakly bound site at 70 < T < 120 K. Neutron diffraction experiments were carried out on CD4/SWCNs to complete this study and determine the packing of the adsorbed solid. It was shown that the methane molecules are aligned along the interstitial channels of the bundles and form a unidirectional solid with a short range order.

2:45 PM AI14
CHEMICAL EFFECTS OBSERVED IN THE SERS SPECTRA OF SINGLE WALL NANOTUBES. M. Bizaran, I. Bilicic, Natl. Inst. of Materials Physics, Bucharest, ROMANIA; S. Leprino, O. Chevreau, J.Y. Mvouelle, IMN, Univ. Nantes, FRANCE; L. Vincenzi, P. Bernier, GDPC, Univ. Montpellier II, FRANCE.

The SERS technique is very successful in the case of SWNTs to amplify the Raman response leading to interesting results such as the asymmetry observed in the Stokes/anti-Stokes spectra of metallic tubes [1]. In our study, we have focused on the strong chemical effects arising at the interface between the nanotube layer and the metallic support. Strong modifications are observed on the Raman spectra, which depend on different parameters such as the nature of the metallic surface, the type of solvent used to disperse the nanotubes and the thickness of the nanotube layer. These results will be discussed in terms of interfacial compounds which induced a strong disorder or defects on the nanotubes. 1. S.D.M. Brown et al, PRB 61, R5357 (2000)

SESSION A12: COMPOSITES
Chair: Al. M. Cassell
Wednesday Afternoon, November 29, 2000
Gran Ballroom (Sheraton)

3:50 PM #A12.1

We have studied the phase diagram of single wall carbon nanotubes stabilized in water by surfactant molecules. Homogeneous dispersions, compact clusters or ramified gels are observed. The phase behavior can be understood by considering surfactant adsorption and depletion interactions induced by the surfactant micelles. When entrained through a capillary tubing in the co-flowing stream of a polymer solution, homogeneous dispersions can be transformed into long ribbons of nanotubes, as shown by electron microscopy. In optical microscopy, the carbon nanotubes exhibit a preferential orientation arising from flow induced alignment. When the ribbons are extracted from water, capillary collapse and water evaporation lead to dense carbon fibers made of entangled nanotubes. The diameter of the fibers can be varied from 10 to 100 microns and their elastic modulus is about 15 GPa, an order of magnitude greater than the modulus of bucky paper. By contrast to more classical carbon fibers, nanotube fibers are highly flexible and do not break even when tightly knotted. This simple and versatile processing may serve in the future for making new fibers with potentially useful mechanical, electrical and electromechanical properties.

4:00 PM A12.2
MULTIFUNCTIONAL CARBON NANOTUBE CHARGE TRANSFER COMPLEXES: STRUCTURAL ACTUATOR, ENERGY STORAGE, AND ENERGY HARVESTING FUNCTIONS. Ray Baughman, Chuanqing Cui, Anver Zhukov, Ilayo Kyarulini, Mikhail Kovol, Honeywell Int., Morris, NJ; Norm Barcik, Geoff Spinks, Gordon Wallace, University of Wollongong, Wollongong, AUSTRALIA; Mark Elwass, Georgetown University, Washington, DC; Leo Fifeled and Larry Dalton, Univ. Washington, Seattle, WA.

The ultimate goal of this work is to provide carbon nanotube composites that provide a structural function together with one or more other key functions, such as electrical energy storage, mechanical and thermal energy harvesting, mechanical actuation, mechanical damping, and sensing. Most of these functions utilize electrochemical double-layer charging injection between ultrastrong nanotube electrodes in an ionically conducting matrix. We describe our efforts to demonstrate and optimize each of these functions. The functions that we have experimentally demonstrated are electro-mechanical actuation, energy storage, electro-chemical thermal energy harvesting, and sensing. These functions will provide the focus of this talk. However, theoretical analysis of other functionalities, and initial experimental work towards their experimental realization, will also be described.

4:15 PM AI13
Raman SPECTROSCOPY OF NANOCOMPOSITES: TEST OF LOAD TRANSFER, INTERFACES, RESIDUAL STRESSES. V.G. Hadjiev, Institute for Space Systems Operations and Texas Center for Superconductivity, University of Houston, Houston, TX; M.N. Blew, Texas Center for Superconductivity, University of Houston, Houston, TX; S. Arek, P. Nikolov, C.B. Tech, Lockheed Martin, Houston TX; B.S. Files, C.D. Scott, NASA Johnson Space Center, Houston, TX.

We report on a Raman scattering test that is used to infer elastic properties of single-wall carbon nanotubes (SWNTs) in composites. The test exploits the strain-induced frequency shift of Raman active modes of SWNTs embedded in epoxy resin subjected to bending. It takes advantage of polarization selectivity of the Raman response: it is dominated by the signal from nanotubes aligned along the laser polarization direction. Polarized Raman spectra are used to distinguish between strain due to pressure effects and that due to direct coupling of SWNTs to the matrix. The strong interfacial stress to failure of the composite is found to create residual stresses on the SWNT ropes. This data is used to estimate load transfer between SWNTs and the matrix.

4:30 PM A12.4
DIELECTRIC SPECTROSCOPY OF CARBON NANOTUBE COMPOSITES. B.H. Fishline, F.W. Howard, DQ. Li, L.S. Li and L.E. Robel, Los Alamos National Laboratory, Los Alamos NM, Z.K. Tang and G. Li, Physics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, PR CHINA.

Theoretical and experimental measurements of the electrical properties of individual carbon nanotubes suggest that they can be used to make interesting dielectric composites for use in capacitors, filters, phase shifters, microwave lenses, electromagnetic shields, and electromagnetic absorbers. However, the processes used to produce these composites such as carbonization could also change the nanotube conductivity and other properties required for good composite performance. In addition, the local environment of a nanotube can change its conductivity dramatically, as has been seen in recent experiments with oxygen adsorption onto nanotube surfaces. Similar effects could occur when nanotubes are suspended in a non-conducting matrix material. Also, room-temperature ballistic electron transport could affect the dielectric properties of composites made with either multivall or single-wall carbon nanotubes. (Although this is for room-temperature ballistic electron transport has been seen only in freely suspended multivall carbon nanotubes.) By fitting the parameters of a Maxwell-Garnett calculation of a composite's complex dielectric constant to frequency-dependent measurements of this quantity, we can determine the number of nanotubes that have been processed to produce a macroscopic volume of composite material. The technique could also allow us to see the effects of ballistic electron transport, if they are present. In our calculations we can use either a classical Drude free-electron model or quantum mechanical models of the nanotube's complex dielectric constant. The technique has allowed us to measure the in situ conductivity of nanotubes suspended in various types of matrix.

4:45 PM A12.5
FABRICATION AND CHARACTERIZATION OF CARBON NANOTUBE-REINFORCED POLYMER COMPOSITES BY ELECTROSPINNING AND SPIN COATING: Yi Yu, Wenzhi Li, Jinhua Chen, Jingwen Wen, Zhifeng Ren, Boston College, Dept. of Physics, Chestnut Hill, MA; Heidi Schroeder-Gibson, Michael Sennett, North Star Soldier Center, US Army Soldier Biological & Chemical Command, North, MA.

Different concentration of carbon nanotubes were added into polymer solution (PEO, PVP, etc.) to form the carbon nanotube-reinforced composites by electrospinning and spin coating. The electrical conductivity and mechanical properties of the composites have been studied. An improvement of at least two orders of electrical conductivity has been observed when carbon nanotubes used in this study has been synthesized by conventional chemical vapor deposition
in a tube furnace. In order to establish the relationship between the concentration, diameter, length of carbon nanotubes, and the properties of the end composites, we have synthesized carbon nanotubes with different diameters and length.

SESSION A13: POSTER SESSION
SYNTHESIS
Wednesday Evening, November 29, 2000
8:00 PM
Exhibition Hall D (Hyatt)

A13.1
SYNTHESIS, CHARACTERIZATION AND APPLICATION OF THIN FILM CARBON NANOTUBE MATERIAL
A.N. Okhissaceous, A.P. Volkov, Faculty of Physics, Moscow State University, Moscow, RUSSIA.

Thin film carbon material consisting of multiwall carbon nanotubes and nanosized graphite crystallites was synthesized using non-cata-

lytical chemical vapor deposition (CVD) process in direct current discharge plasma activated by methanol-hydrogen gas mixture. A low-threshold field of 1.5 V/μm, high-emission current and size densities of 100 mA/cm² and 10⁷ cm⁻², correspondingly, for an applied field of 5 V/μm were achieved. It was established by using high-resolution electron microscopy that graphite sheets composing these nanotubes and graphite-like crystal layers have predominant orientation along a normal to the film surface. X-ray and UV-radiation spectroscopy exhibit in the films carbon clusters characterized by low work function. Cathodoluminescence at around 4 eV and 2 eV was also observed for the CVD films. This combination of experimental observations is explained by specific structure of obtained graphite-like material with curved atomic layers having modification of electronic properties due to rehybridization of atomic bonds. Applicability of the CVD films are demonstrated by fabrication of flat panel display prototypes with diode and triode configurations.

A13.2
DECORATED NANO-TUBULAR STRUCTURES DEPOSITED BY HF-CVD
Ralph Kurt, Aydonal Kurmi, Swiss Federal Institute of Technology (ETHZ), Dept of Physics, Lausanne, SWITZERLAND.

A hot filament chemical vapour deposition (HF-CVD) process was used to synthesize a new type of nitrogenated carbon tubes. The structure and the chemical composition of the deposits grown onto pure Si wafer were studied by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS). Spherical agglomerates, twisted nitrogenated carbon fibers, chains of nanobeads, and coiled nanotubes were produced in a controlled way which shape, diameter and length depend on the interatomic distance from the filament. All these tubular structures show an interesting feathered surface. A possibly interpretation of the observed growth perpendicular to the tube axis regarding to the influence of Nitrogen in the structure will be given. The crystallinity of the structure is derived from the electron diffraction pattern and the lattice planes clearly seen in high resolution (HR) TEM. The nanotubes seem to be hollow. The question, if the tubular structures growth auto-catalytically or is possibly influenced by any tungsten carbides acting as catalysts will be discussed. The optical vibrational properties were analysed by Raman spectroscopy showing the typical disordered graphitic bands. Additionally an unidentified peak at 1800 cm⁻¹ was observed and the G-Peak was decomposed into two sharp but overlapping peaks. This might be interpreted in terms of two different growth mechanisms resulting in the decorated tubular structures. The large surface area might make the material interesting for any catalytic application or for mechanical composite materials.

A13.3
ON THE ROLE OF THE PRECURSORS IN THE EARLY STAGES OF NANOtube NUCLEATION
Dario Nardacci, Istituto Nazionale per la Fisica della Materia and Dept. of Materials Science, University of Milano Bicocca, Milano, ITALY; Barbara Mariangeli, Dept. of Materials Science, University of Milano Bicocca, Milano, ITALY; Paolo Milani, Istituto Nazionale per la Fisica della Materia and Dept. of Physics, University of Milano, Milano, ITALY.

A study will be presented on the role of chemicals in Aerosol-Assisted Chemical Vapor Deposition (AACVD) of carbon nanotube [NT] films. Attention has been paid to the effect of different precursors on the growth rate and on the graphite/nanotube ratio. NTs were nucleated onto oxidized Si wafers at temperatures between 560 and 650 °C by co-depositing NO and CO from a solution containing Si acetate and different organic chemicals. Films were eventually annealed up to 800 °C in Ar. Micro- and macro-Raman spectra were used to identify the presence and the relative abundance of NT structures. It will be shown how the choice of proper organic precursors must be optimized accounting for the interplay between the organic catalytic decomposition temperature (which is generally different from the so-called thermodynamic decomposition point) and the critical temperature separating the thermodynamically-controlled and the catalytically-controlled growth regimes. High temperature decomposing chemicals will display a stronger tendency to nucleate graphitic NTs, inhibiting the possibility of sufficiently growing NT films at low temperatures. At the same time we will show how the chemicals restrict the growth of NTs at low temperatures lower than 500 K by using plasmonic precursors, while it will be shown how different organic precursors cannot be used under the same deposition conditions to obtain NT films.

A13.4
ENERGY BARRIERS AND NORMAL MODES IN ROLLING OF GRAPHENE FRAGMENTS INTO CARBON NANOTUBES
Manuel Velpe, ENEA, Divisions Materiali, Centro Ricerche Canevizza, and Dip. Science e Tecnologie Chimiche, Università Tor Vergata, Roma, ITALY; Fabrizio Clari e Gregorio D'Agostino, ENEA, Divisione Materiali, Centro Ricerche Canevizza, and INFN, Roma, ITALY; Vittorio Zanotto, ENEA, High-Performance Computing Project, Centro Ricerche Canevizza, and INFN, Roma, ITALY.

We present a theoretical study of the nucleation mechanism of carbon nanotubes based on the hypothesis that the starting nanotube seed can be nucleated by rolling a small fragment of a graphene sheet (graphene) under thermal fluctuations. The energy barriers for rolling a graphene along different crystallographic directions are calculated from a tight-binding model, and are plotted as a function of the curvature radius of the nanotube. This allows to establish a universal energy scale for each family of nanotubes. The effect of introducing an increasing number of pentagonal rings in the flat, hexagonal graphene structure is investigated. We then estimate the amplitude of the fluctuations and the vibrational modes of graphene sheets of increasing size by means of tight-binding molecular dynamics simulations at very high temperatures. Such a model can be representative, e.g., of the high-temperature ablation of graphene fragments during arc discharge experiments. We discuss the combined effects due to: (a) the decrease of the energy barriers against rolling with increasing nanotube radius, and (b) the increase of random fluctuations with increasing size of the graphene sheet. The superposition of such effects may lead to a preferential range of nanotube diameters which could nucleate more abundantly than others. Work performed under the Project PRID5001110 “Innovative Materials Based on Carbon Nanotubes” of the Italian Space Agency (ASI).

A13.5
SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF CARBON NANOTUBES PREPARED BY ARC DISCHARGE UNDER LIQUID NITROGEN
Marco Vittori Antici, Renzo Munazzi, Francesco Cardellini, Vittoria Contini, Fabrizio Clari, Manuela Velpe, Roberto Conversano, ENEA, Centro Ricerche Canevizza, Roma, ITALY.

Carbon nanotubes prepared by arc discharge performed under liquid nitrogen have been characterized by X-Ray diffraction, transmission electron microscopy and electron energy loss spectroscopy (XRD and EELS) spectra were also simulated by means of tight binding molecular dynamics simulations. The effect of the processing conditions and particularly the DC voltage across the discharge, on the quality of the resulting carbon nanotube structures has been assessed. The raw material has been purified following the classical route of selective oxidation in nitric acid. Multiwall nanotubes with very clean and defect-free surfaces, was observed for a applied voltage of the order of 22 V. On carbon rods 5mm in diameter the DC current resulted of the order of 20 A. The method is very simple, at the same time allowing to show a high yield with productivities of the order of grams/hour of raw material; furthermore it can be scaled to even larger scale in the near future without any conceptual difficulty. By contrast when the voltage was raised to about 30 V, with a current of about 25 A, the rough material shows a diffraction pattern with a very reduced intensity of the 002 graphite peak, suggesting the presence of nanotube structures based on graphite monolayers; the relative TEM image shows a complex and heavily convoluted microstructure whose identification requires further work currently in progress.

A13.6
CALCULATION OF NANOTUBE CONTENT IN ARC PRODUCED CARBON POWDER USING ELECTRON PARA MAGNETIC RESONANCE
Department of Physics, University of Dublin, Trinity College, Dublin, IRELAND.
We have described a method that maximizes the phase separation of turbostatic graphite (TSG) and multi-walled carbon nanotubes (MWNT) in solutions of various organic polymers. This involves the formation of sediment and a solution. These components were characterized for MWNT and TSG content using electron paramagnetic resonance (EPR) measurements. All EPR samples could be deconvoluted into nanotube and TSG components. When normalized, these components are representative of the mass of MWNT and TSG present. This allows us to make quantitative measurements of nanotube and TSG content in different environments. The most successful polymer host was poly(m-phenylene-co,2,5-fluorenylene-1,4-phenylenevinylene) (PPvFV). Using thermogravimetric analysis to calculate the mass of nanotubes in host film we could calculate an EPR signal intensity per unit mass. By comparing this to the signal intensity of the nanotube component in the crude powder we could calculate for the first time the nanotube content or purity of our produced nanotube powder.

A13.7
CONTROLLED GROWTH OF CARBON NANOTUBES BY CHEMICAL VAPOR DEPOSITION. Z. Li, D.Z. Wang, S.X. Yang, J.G. Wen, Z.P. Ren, Department of Physics, Boston College, Chestnut Hill, MA.

Carbon nanotubes have been synthesized directly on graphite foil coated with stainless steel film with thickness ranging from 2 to 100 nm by chemical vapor deposition. The catalyst particle size increases with the thickness of the stainless steel film. The diameter, the number of walls, and the purity of the carbon nanotubes are controlled by the catalyst particle size. Transmission electron microscopic examination reveals that the carbon nanotubes are well graphitized and consist of 3 to 20 graphite layers depending on the catalyst particle size. The result indicates that it is possible to synthesize required carbon nanotubes by tuning the size and distribution of the catalyst particles in the chemical vapor deposition process.

A13.8
DIRECTED GROWTH OF NANOTUBES USING MICRO-CONTACT PRINTING OF CATALYSTS. Jeong-Ki Shin, Young-Soo Han, Sung-Tae Kim, LG Electronics Institute of Technology, Innovation Center, Seoul, KOREA.

The directed growth of suspended nanotubes is essential for CNT device applications. It is well known that self lithography is a very useful technique in many applications. In the present work, selective growth of carbon nanotubes in orientation parallel to substrate, was attempted by microcontact printing. Synthesis of structurally perfect nanotubes has been demonstrated by an acetaldehyde CVD method. We observed that the morphology and growth rate were strongly dependent on the acetylene gas flow rate, the fraction in diluted reaction gas and temperature. These results will be discussed in terms of reaction kinetics of CVD process.

A13.9

Single-walled carbon nanotubes (SWNTs) have recently been considered as a new class of electronic materials because of their ultra narrow tube diameters and unique electrical properties, which are strongly dependent on their diameters and chirality. SNTNs are easily produced by arc discharge method which results in extremely long, highly tangled nanotubes. They also contain large amounts of impurities such as amorphous carbon and catalytic metal impurities which should be removed for their advanced applications, thus, the development of a suitable method for purification and separation of SWNTs is crucial for further progress on nanotubes. SWNTs were reacted with typical oxidizing acids such as nitric and sulfuric acid and were ured in an ambient of H2O2 to minimize damage on the tips of acid-treated SWNTs. By such chemical oxidation, raw SWNTs were purified and cut into short lengths, which was confirmed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy dispersive spectrometry analysis (EDS). The purified SWNTs were classified into different sizes by the Field Emission Phenomena (FEP) method. The length of SWNTs were more uniformly distributed after acid treatment and it is estimated that SWNTs are cut into short lengths of less than 2 μm. Moreover, field emission characteristics of purified SWNTs were investigated to study the effect of purification on the field emission. The purified SWNTs were uniformly deposited onto patterned ITO electrodes by electrophoresis. A turn-on electric field was 6.7 V/μm, where an emission current was uniformly maintained to be 10 μA/cm² as long as 800 min. In this study, the effects of purification and size distribution on the field emission will be discussed.

A13.10
EFFICIENT OF ULTRAFINE GOLD PARTICLES AND CATIONIC SURFACTANT ON BURNING OF AS-GROWN SINGLE-WALL CARBON NANOTUBES. Minfeng Zhang, Minako Yudawa, Fumihiko Nihy, Sumio Iijima, ICORP-JST, NEC, Tuskuba, JAPAN, Meijo Univ., Dept. of Physics, Nagoya, JAPAN.

A simple method of purifying single-wall carbon nanotubes (SWNTs) proposed so far is gas-phase oxidation; but amorphous carbon (a-C) and graphitic are difficult to remove because the temperatures are close to that of SWNT. Other purification methods using strong acids can remove a-C, but the acid is thought to damage the SWNTs. Recently, Mizoguchi et al. [1] have shown that a-C in as-grown SWNTs can be removed by oxidation at lower temperatures by using ultrafine gold particles and a cationic surfactant benzalkonium chloride (BKC). In this purification, SWNTs remain less damaged than in the former two purification methods. In this study, we used thermogravimetric analysis (TGA) to investigate the effect of ultrafine gold particles and the cationic surfactant on the burning of the various carbonaceous materials contained in as-grown SWNTs. We found that the ultrafine gold particles catalyzed the oxidation of carbonaceous materials leading to a decrease in its burning temperatures, and BKC played the role of homogenizing the a-C aggregation states, which resulted in a-C burning in a narrow temperature range.

A13.11

Carbon nanotubes have been deposited by electrophoresis for field emission display (FED) devices. Single-walled carbon nanotubes (SWNTs) were used after purification. A solution for the electrophoresis was prepared by dispersing the SWNTs, surfactants, charging, water, and so on. Carbon nanotubes (CNTs) were selectively deposited on 5.6-inch patterned ITO glass substrates. The deposition was optimized by computer simulations for different line and space widths, which agreed well with experimental results. Better deposition behavior was observed at smaller line widths for a given line pitch due to concentration of higher electric fields at the line edges. In case of the 60 μm wide line and 98 μm wide space, the electrophoresis was optimally carried out at 2040 V for 20 sec for the electrode distance of 5.0 mm. A turn-on electric field was approximately 0.60.7 V/μm and uniform emission of 10-14 A/cm² for an extended time of 800 min was achieved at 2V/μm. The CNT cathode deposited by electrophoresis showed lower outgassing than that of the screen-printed CNT cathode after vacuum packaging. The electrophoresis of CNTs showed its simplicity of fabrication processing and excellent field emission characteristics for the application in FEDs. We also fabricated a triode type field emission display using the cathode placed with CNTs deposited by electrophoresis. Main factors to control electrophoresis of CNTs, its optimal process conditions, and fabrication processes for FED applications will be discussed in detail.

A13.12
FORMATION OF CARBON NANOTUBES BY USING RF PLASMA CVD EQUIPMENT FROM METHANE, ACETYLENE AND HYDROGEN GASES. Yoshiyuki Show, Toshihito Matsukawa, Mitsuo Iwase and Tomio Iizumi, Department of Electronics, Tokai University, Hirano, Kita-ku, JAPAN.

Carbon nanotubes (CNTs) are promising material for cold cathode in the field emission display. The CNT is formed by the thermal and microwave-plasma CVD methods. However, these synthetic methods are difficult to form the CNTs on large substrates. In this presentation, we will report the synthesis of the CNTs on the SiO₂ film by the radio frequency (RF) plasma CVD method at temperatures below 100°C. This CVD method has the advantage of formation of the CNTs on large substrates. The SiO₂ film (thickness of 1000 nm), formed on the Si substrate, was used for the substrate. The round Ni particles with the size of 50 nm were deposited on the SiO₂ film for the nucleation of the CNTs. The CNTs were synthesized by the microwave CVD method (100 W, 2.45 GHz). The CNTs were synthesized by the microwave CVD method (100 W, 2.45 GHz). The Ni is reduced by the hydrogen (H₂) gas. Typical condition of the gas was 0.6 and 10 sccm for the CH₄ and H₂ gases, respectively. The chamber pressure and the RF power during the deposition were kept at 1x10⁻² Torr and 50 W, respectively. The deposition time was varied from 10 to 30 min. The depositing rate of the carbon was kept below 100°C. The SEM observation
showed that the CNTs with average diameter of 10 nm were synthesized on the Na-particle-coated SiO2 films at the above mentioned decomposition condition. The CNTs were almost randomly formed on the large area of 50x50 mm. The density and length of the CNTs were increased with the deposition time. The average length of the CNTs were synthesized for 30 min., was 500 nm.

A13.13
NATURE OF A FIELD-EMISSION FROM CARBON NANOTUBE FILMS. Zina Konkovskaya, Yuri Gulyayev, Tat'yana Pyshnaya, Anna Konkovskaya. Moscow State Technical Engineering and Electronics of RAS, RUSSIAN FEDERATION.

Now carbon nanotube structure are considered as an extremely perspective material for tubes of high field displays. This interest is caused by high field emission from nanotube structures [1,2]. It's known, the stability of field emission is very important characteristic for practical application of nanotube in flat display, but till now this problem not completely solved. The reason of this is absence of understanding of the mechanism of occurrence of high field emission from these structures. In our work we studied the features of emission properties of carbon nanotube films. The object of our researches were a well-oriented carbon nanotube films on substrates of silicon, quartz and nickel, which were synthesized by electron beam method [3]. The analysis of current - voltage characteristics of field emission [VAX] has shown impossibility of the full description this phenomenon by Fowler-Nordheim tunneling mechanism. Fowler-Nordheim tunneling mechanism does not give answers to the following questions: Why density current of field emission from nanotube films is higher than we have by calculation? Why have not a threshold of saturation? The threshold of saturation is extremely important characteristic for practical applications nanotube films in flat display. Why at critical current we observed a destruction of nanotubes without substantial increase of temperature of substrate? What is mechanism? In this work we offer a new mechanism of field emission which takes into account as a geometry of nanotip, as well as peculiarities of carrying a charge in them. This work was supported by RFBR under Grant 09-03-17310. I. Gulyayev Yu.V., et al. Revue LE Vide et Cogher Minors' Supplement n.z N271 - Mars-April 1994 (7th Int. Vacuumconf, 94, Grenoble, France) P.222-236. 2 V.A. de Heer et al. Science, 1995, 260, 1117 3. Konkovskaya Z.V. JETP Lett. 1999, v.56, No.1, pp.26

A13.14
SELECTIVE GROWTH OF ALIGNED CARBON NANOTUBES ON SiO2/Si PATTERNS FROM XYLENE METALLOCENE MIXTURES. Z.J. Zhang, B.Q. Wei, G. Romannat, P.M. Ajayan, Rensselaer Polytechnic Institute, Department of Materials Science and Engineering, Troy, NY.

Growing 3D networks of aligned carbon nanotubes on flat substrates by a bottom-up approach is important to harness the unique electronic properties of carbon nanotubes for device applications. Sematic control over nucleation sites and growth direction essential to realize nanotube architectures remains a challenge. Here, we report a new method for growing aligned carbon nanotubes selectively on SiO2 surfaces by chemical vapor deposition from xylene-metallocene mixtures. This approach obviates the use of metal catalyst films, thus providing an easier way of selectively growing nanotubes on Si substrates through standard device processing methods. SiO2 patterns on Si, obtained by lithographic patterning and thermal oxidation, or (001) substrates, were exposed to xylene-metallocene mixtures at 800°C. Scanning and transmission electron microscopy [SEM and TEM] of SiO2/ Si patterns after deposition reveal the selective growth of vertically aligned multiwalled carbon nanotubes on SiO2 surfaces. There is no observable nanotube growth on the Si surfaces. This interesting growth behavior may be used to realize 3D architectures of carbon nanotubes for applications in nanodevices. Based upon the above, we have developed a general approach to control the nucleation sites and growth of the nanotube patterns, we proposed a phenomenological model to explain the mechanism of selective growth and alignment of nanotubes.

A13.15

The preparation of highly anisotropic 1D structures confined into single walled carbon nanotubes is one of the key objectives in carbon research, as the introduction of these materials into the hollow nanotubes creates unique properties due to interference effects on their optical and electronic properties. We report here the filling of single and double walled carbon nanotubes by two different p-block halides, TICI and PH2. LE. The nanotubes were produced either by the arc synthesis [1] or by chemical vapor deposition technique [2], based on the reduction of a MgCl2 solid solution by a Hydrogen-Methane mixture. In the case of TICI, the structure of the crystals observed inside the tubes were all found to be derived from the rodshaped form and bi- and trilayer crystals were observed. We also report the growth of a Perovskite phase relative to the for structure, as determined from HRTEM. In contrast, the crystal structure of bulk TICI is a C6c2 type structure. These results are consistent with the recently reported reduced coordination K12 compound formed within SWNT [3]. The C6c2 (C1c2 crystal structure), the use of HRTEM image simulations will be combined to the characterization by XAS and core level XPS to confirm the coordination of Pb atoms in the 1D confined structure. The confined Pb12 compound forms a 1D array of reduced coordination polyhedra formed within the SWNT capillaries. [1] C. Journet, W.K. Minser, P. Beccher, A. Loiseau, M.L. de La Chapelle, S. Lefranc, P. Der Nézi and E.E. Fischer. Nature 388 (1997) 78. [2] E. Flahaut, A. Pagny, Ch. Laurent, A. Raveau, J. Mater. Chem., 10, 2000, 249 [3] J. Sloan, M.C. Novotny, S.R. Bailey, G. Brown, C. Xu, V.C. Williams, S. Friedrichs, E. Flahaut, R.L. Callendre, A.P.E. York, K.S. Coleman, M.L.H. Green, R.E. Dunin-Borkowski and J.L. Hutchison. Chem. Phys. Lett., in press.

A13.16
SYNTHESSES OF SINGLE WALL CARBON nanotubes UNDER HIGH MAGNETIC FIELD BY ARC DISCHARGE. Haruo Yokomichi, Toyama Prefectural Univ, Dept of Electronic and Informatics, Toyama, JAPAN; Mitsuaki Ichihara, Fumiko Sakai, Univ of Tokyo, Inst for Solid State Physics, Chiba, JAPAN; Kikuo Ichih, Naoki Kishimoto, National Research Inst for Metals, Tsukuba, JAPAN

Morphological control of carbon nanotubes as well as the bundle aromaticity is important in applications of the nanotubes to practical devices. Recently, we have reported the synthesis of multi wall carbon nanotubes under high field up to 10 T in order to achieve morphology control of nanotubes [1]. In the present study, synthesis of single wall carbon nanotubes was attempted under high field of 10 T by arc discharge. The arc discharge was carried out under a current of 40 A in a He gas atmosphere using the graphite composite rod for the anode. The composite rods were prepared by burning a 5-mm diameter hole at the end of a 5-mm diameter carbon rod and the hole was filled with a mixture of graphite, Fe and Ni powder with 95.25.7.5.2.5 (w/w). The rod was annealed in a vacuum of approximately 0.01 mTorr at 950°C for 1 hour. Synthesized catalyst deposit and soot were investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). From TEM images, it was confirmed for the first time that single-wall carbon nanotubes form in the carbonode under a magnetic field of 10 T. This result corresponds to the fact that the carbonode deposit synthesized under 10 T contain Fe and Ni catalytic metals, whereas these synthesized without magnetic field do not contain these metals. The radius of nanotubes synthesized under 10 T is larger than that without magnetic field. Furthermore, the yield of the former nanotubes seems to be larger than that of the latter nanotubes. Based on these results, effects of magnetic field on synthesis of nanotubes are discussed. [1] H. Yokomichi, H. Sakima, M. Ichihara, F. Sakai, K. Ichih and N. Kishimoto, Appl. Phys. Lett. 74, 1827 (1999)

A13.17
COMPUTATIONS OF nanOTUBES RELATED TO C60. Zdenek Shiming, Department of Knowledge-Based Information Engineering, Tohoku University of Technology, Tohoku, JAPAN; Filip Ulibik, Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, CZECH REPUBLIC; Filip Jurečka, Department of Knowledge-Based Information Engineering, Tohoku University of Technology, Tohoku, JAPAN.

Recently, Sun et al. (Nature 403, 384, 2000) reported the narrowest carbon nanotubes so far and suggested that it could be closed by a half of a C60 cage. The present paper reports computations on related model systems. There is a symmetric cut of D6h C60 cage with six pentagons and model nanotubes with such cap were derived. One can also cut the D2d C60 cage and thus create another cap and D2d-related model nanotubes (this patch can also be obtained from the D6h cage). There is a clear difference in the energies of the two nanotubes. For example, as the PMI computational level in a reduced C60 representation, the D2d-related model nanotube is lower in energy by some 775 kJ/mol and has in its middle a diameter of about 5.42 Å (the D6h-related model nanotube about 4.81 Å). This computed model geometry corresponds well with the experimental value of 5 Å reported by Sun et al. (Nature 403, 384, 2000). Various modelling approaches are to be discussed in the paper.

A13.18
COLLOIDAL SOLUTION OF METAL nanoparticles AS A CATALYST FOR CARBON nanOTUBE GROWTH. Hieko Ayo, Satoshi Oshima, Tatsuki Komatsu, Yasuori Kuriki, Motoo Yamur, National Institute of Materials and Chemical Research (NIMC), Tsukuba, JAPAN; Jumpei Fine Ceramics Center (JFCC), Tokyo, JAPAN.

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A method to synthesize carbon nanotubes, chemical vapor deposition (CVD) in the presence of a transition metal catalyst has attracted interest because of the CVD process at relatively lower temperature with less carbon impurities and gives much larger quantities compared with other methods. In the CVD method, metal nanoparticles are essential for the growth of carbon nanotubes, because they act as a catalyst for the nanotube growth; the size and chemical composition of the metal nanoparticle determines diameter and structural perfection of the nanotube. Metal nanoparticles employed in the CVD reaction have been realized mainly by using nanoparticles supported by etching or laser ablation. For better development, a more simple synthetic method applicable to plane and large area substrates is very important. In this paper, we show that metal nanoparticles of average diameter of 1.5 nm chemically synthesized by a reverse micelle method catalyzes the growth of multi-wall carbon nanotubes (MWNTs). The surface of the nanotubes is covered with surfactants so that the nanoparticles can be dispersed in organic solvent and, thus, highly processable. Thermal CVD reaction of methane in the presence of the catalyst film of the dispersion on a plane Si substrate resulted in the MWNT array aligned perpendicular to the substrate. This array of the MWNTs has potential applications, especially to field emission displays, because the density of the present MWNT array is relatively low and the array can be developed to large area. We also show that the colloidal dispersion of the metal nanoparticles can be applied to the vapor-phase reaction in a hydrogen flow, which produced a large quantity of carbon nanotubes. Through the control over the diameter and chemical composition of the nanoparticles, we may be able to control the diameter and chirality of the nanotube in the near future.

A13.19 SYNTHESIS OF CARBON NANOSTRUCTURE BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION OF Fe-PD/THERALOC/AVEE: Takahiro Imai, Shin-ichi Honda, Tatsuki Oyama, Yong-Gyu Baek, Shigeharu Okura, Masahiro Kitagawa, Kenjiro Osuna, Department of Electronic Engineering, Graduate School of Engineering, Osaka University, Osaka, JAPAN; Jung-Tak Ryou, Department of Computer and Communication Engineering, Pohang University, Kyungbok, KOREA; Masahiko Kitagawa, Shinko-seiki Corp., Kobe, JAPAN.

Recently, carbon films with nanostructure have been attracted due to their property of cold cathode materials for flat panel display applications. The low temperature process for display has been required because glass materials would be used as the substrate. We have established low temperature synthesis a carbon nanostructure. The carbon nanostructure was formed using plasma enhanced chemical vapor deposition on Si(100) and glass substrate at 400°C. Plasma was generated between W filament and anode electrode at 728.1×10³ Torr of Ar atmosphere. Fe phosphocyanide (FePc; FeC3H4N2) was used as a source material, which can supply Fe, C, H and N. FePc was positioned on anode electrode, which was sublimated by plasma and formed carbon nanostructure on substrate. The formed carbon nanostructure was analyzed its surface morphology, internal structure, and crystalline structure by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD), respectively. The general feature of the nanostructure has fiber-like shape with 18-100nm diameter and 1-10μm length. The fibers were oriented randomly but were grown with high density. This nanostructure was crystalline graphite determined by X-ray diffraction measurement. High vacuum chamber was used to measure the field emission from these carbon nanostructure. The density of emission current J reached a value of 0.1mA/cm² at a turn-on field of about 3V/μm which was remarkably efficient electron emission current at a low field in comparison with other carbon related field emitters. More detailed results of structural analysis and emission properties for the nanostructure will be reported.

A13.20 GROWTH OF CARBON NANOTUBES ON CARBON CLOTH. W. Z. Li, J. G. Wen, Z. P. Ren, Department of Physics, Boston College, MA.

Up to now, carbon nanotubes can be easily prepared on many kinds of substrates, such as silicon and glass, by different methods. However, it is still a main problem to synthesize large area of carbon nanotubes on flexible and conducting substrates. In this contribution, a significant advancement has been developed to synthesize large area of carbon nanotubes on iron nitrate silicon gel coated carbon cloth using chemical vapor deposition. The catalysts of the nanotubes have uniform diameter and high purity. The density and uniformity of the carbon nanotubes are dominated by the substrate preparation and growth condition. Carbon nanotube film grown on the carbon cloth can be easily adapted to meet different applications.

A13.21 LITHIUM INTERCALATED SINGLE WALL CARBON NANOTUBES. Hideki Shimoda, Xiaoping Tang, Bo Guo, Alfred Kleinschmidt, Leslie Fleming, Yue Wu, Otto Zhou, Univ. of North Carolina at Chapel Hill, Dept. of Physics and Astronomy, Chapel Hill, NC.

SWNTs fabricated by the laser ablation method were purified and reacted with lithium via solid state and electrochemical methods. 13C NMR measurement shows that the spin-lattice relaxation times (T2) of the single-wall carbon nanotubes become shorter after reaction with Li, indicating the increase of the electronic density of state at Fermi level due to charge transfer. Crystalline X-ray diffraction pattern similar to that of the pristine materials was observed from Li reacted SWNTs. Purified SWNTs were also cut into short bundles by the oxidation method. The effects of nanotube structure/morphology on the intercalation kinetics will be discussed.

A13.22 FABRICATION OF FREESTANDING CARBON NANOTUBE ARRAYS IN LARGE SCALE. Z. P. Heng, J. Moser, M. Sennett, H. Gibson, M. J. Naughton, and Z. P. Ren, Boston College, Dept. of Physics, Boston, MA.

We have successfully fabricated many freestanding carbon nanotube arrays on a silicon substrate. Different sizes of dot arrays have been made by E-beam lithography. It has been found that the size of the carbon nanotubes is closely related to the size of the dot. Compared with our previous report on diameters of about 300-400 nm, much thinner carbon nanotubes of 100-150 nm have been made. With even smaller dot, it would be expected that even thinner nanotubes of 10-20 nm can be possibly made. The nanotube height was controlled by the growth time. Height uniformity has been greatly improved.

A13.23 THE ACCURATE CONTROL OF THE DIAMETERS OF CARBON NANOTUBES WITH TRI-LAYER CATALYSTS. Tong-Ryung Choi, Hyuck Ihm, Byung-Dong Kim, Weon-Chul Chang, Yong-Chul Kim and Seung-Ki Joo, Seoul National Univ, School of Material Science and Engineering, Seoul, KOREA.

Recently, carbon nanotubes are in the center of intense interests due to their promising physical properties. These carbon nanotubes can be used in many applications. In each application, different properties and sizes are required. It is well known that the diameters of nanotubes are controlled by surface roughness or morphology of catalytic islands. So many attempts have been made to control diameter by various kinds of methods. However, such efforts have been unsatisfactory because conventional methods can provide only the tendency of changes, not the means of an accurate control. We propose here that a novel accurate method to control the size of carbon nanotubes by means of annealing temperature, time and thickness of layers. When the sandwich-type tri-layer structure of Ag/NiFe/Ag or Au/NiAg/Au is used as a catalyst and annealed, NiFe or NiAg is transformed into the island of expected size depending on the thickness of each layer and the heat treatment condition. In this method, we can change the spacing of catalytic islands as well as the size of them. After the formation of catalytic islands, carbon nanotubes are produced by Hot-filament CVD method. SEM, TEM and Raman spectroscopy are adopted as analytical tools. In addition to the detailed discussion on the results, the synthesis procedure of carbon nanotubes will be also described.

A13.24 STUDIES OF COMPATIBILIZATION OF POLYSTYRENE AND POLY(METHYL METHACRYLATE) WITH MS2 NANO TUBE. W. Zhang, Y. Wang, H. White, M. Rafaiaoldc, J. Sokolov, State University of New York at Stony Brook, Dept of Mat Sci & Eng, Stony Brook, NY; R. Tenne, Weizmann, Institute Rehovot, ISRAEL; A. Ulman, M. Shafi, Chemistry Dept, Polytechnic University, Brooklyn, NY; A. Winesett, H. Aide, Dept Physics, North Carolina State University, Raleigh, NC.

MS2 nanotubes were functionalized with thiol and dispersed in polystyrene and poly(methyl methacrylate) toluene solution. The mixture was spun cast onto Si Surface and the film were examined with Scanning Transmission X-ray Microscopy and Scanning Force Microscopy as a function of annealing time at 170°C. The results showed that the addition of nanotubes decreased the domain size and the contact angle between the polymer. This indicate that the nanotubes are effective at decreasing the interfacial tension between the components and can serve as potential compatibilizers. Banded in part by NSF-MSEC Program and the Proctor & Gamble Co.
A13.25 SELF-ASSEMBLED ORGANIC NANOTUBES. Richam Perniki, Purdue University, H.C. Brown Chemistry Laboratories, West Lafayette, IN.

The universal importance of non-covalent forces in the assembly and stabilization of biological systems provides a compelling motivation to consider a new type of organic synthesis based on these interactions. The challenge lies both in the chemical design and synthesis. The conceptualization of an organized state of matter is intimately linked with the development of the molecular building blocks and the surrounding medium in the form of charges, dipoles, and other functional elements necessary to translate chemical information into substances. Much of the research endeavor has been devoted to the use of the hydrogen bond as the alphabet for chemical information encoding, and the structures expressed have spanned the range of dimensions and shapes, from discrete to infinite networks. The starting point of this research theme is a DNA mimic in which the hydrogen bonding array of the bases as well as the familiar backbone structure is chemically mediated so that the structural outcome of this bio-inspired material is a six-stranded rather than a double-helical assembly. The specific molecular recognition properties of six alternating triminoglycine (TAP) and barbituric acid (BA) molecules, through a set of six hydrogen bonds per unit, can be chemically encoded so that structural outcome is a six-membered supermolecule. Over the past two years we have developed a synthetic strategy to incorporate TAP and BA into oligomeric strands. As a result, their propensity to self-assemble and self-organize into well-defined hydrogen bonded supermolecules was conferred upon the oligomers to which they were attached. This self-assembled framework can be compared to the DNA double helix except that it has a different backbone, six strands instead of two, and defines a built-in channel with predetermined dimensions. Each level of the sextuple helix involves six sextuple helical units [3 TAPs, 3 BA's, eighteen hydrogen bonds] and is engaged in stacking interactions with one or two neighboring plates.

A13.26 STRUCTURE-TUNABLE CARBON MATERIALS FROM GRAPHITE COMPOUNDS. Gong Kecheng, Wang Weixing, Polymer Structure & Modification Research Lab, South China University of Technology, Guangzhou, CHINA.

The discovery of carbon nanotube, nanorod, nanosphere, nanowire etc. has stimulated intense scientific investigations because of their special properties and potential applications. But, how to achieve such nanomaterials in large quantity by some simple and inexpensive fabrication method is challenging. Here we report a novel method of preparing structure-tunable carbon materials from graphite compounds. Graphite compounds such as graphite intercalation compounds, graphite oxide etc. are subjected to heat treatment at various temperature to obtain structure-tunable carbon materials. The intercalation guests and catalyst have great influence on the morphology of the carbon materials. Some TAPs [Tetra-alkyl-pyridine] were used [not limited to] electrode materials for supercapacitors.

A13.27 SELECTIVE FORMATION OF CARBON NANOARCHITECTURE BY CO\(_2\) LASER VAPORIZATION AT ROOM TEMPERATURE. Daisuke Kasaya, Faculty of Science and Technology, Meijo University, Nagoya, Aichi, JAPAN; Kunimitsu Takahashi, Ryoji Koliki, Institute of Research and Innovation, Kashima, Chiba, JAPAN; Masuo Yudawa, "Nanotubulites" Project, Japan Science and Technology, c/o NEC, Tsukuba, Ibaraki, JAPAN; Sumio Iijima, Faculty of Science and Technology, Meijo University, Nagoya, Aichi, JAPAN; "Nanotubulites" Project, Japan Science and Technology, c/o NEC, Tsukuba, Ibaraki, JAPAN.

Single-wall carbon nanohorns (SWNHs) [1] can be produced with a yield of about 20-30% by laser ablation of graphite ribbons at room temperature. An SWNH is a horn-shaped sheet of single-walled graphene sheets with a diameter of 2-3 nm, and they form an aggregate shaped like the flower of a dahlia having a diameter of about 100 nm. The ethanol adsorption capacity of the dahlia-shaped aggregates was considerably larger than that of the commercially available activated carbon [2]. Besides the dahlia shaped aggregate, there are two more types that are called bud-like and seed-like SWNH aggregates. So far we have been unable to study their adsorption capacities because of their low yields. Recently we have found that the type and pressure of the buffer gas could control the aggregate structure. When 760 Torr of Ar gas was used, dahlia-shaped aggregates of about 100 nm were formed. When 760 Torr of He gas or N\(_2\) gas was used, bud-like aggregates with diameters of about 70-100 nm were formed. Seed-like aggregates with diameters of 60 to 70 nm were produced with Ar gas pressure of 360 Torr. To elucidate the mechanism of the effect of buffer gas on the SWNH structure, we clarified the yields of C\(_{24}\) contained in the SWNH. The C\(_{24}\) yield was large in He and low in Ar and N\(_2\), and it decreased with increasing buffer gas pressure. These results do not correspond to the commonly explained formation dependence of SWNHs, so our results require a new model. References [1] S. Ejima et al., Chem. Phys. Lett., 309 (1999) 165. [2] J.A. Nishara et al., Chem. Phys. Lett., in press.

A13.28 GROWTH OF CARBON NANOTUBE FROM VAPOR PHASE. Y.M. Chen and Jyh-Ming Ting, Department of MSE, National Cheng Kung University, Tainan, TAIWAN.

Multi-wall carbon nanotube (MWCNT) was prepared via a chemical vapor process. This process not only allows the growth of MWCNT with less "thermal carbon" but also has the potential for cost-effective production of MWCNT. In the study, we investigated effect of substrate preparation, vapor phase composition, and temperature on the characteristic of MWCNT. The microstructure was determined using transmission electron microscopy (TEM) and the surface morphology was examined using scanning electron microscopy (SEM). The growth kinetics and the variation of microstructure along the tube radial direction were investigated. The substrate preparation was found to be critical to the successful growth of MWCNT. The growth rate of MWCNT increased and then decreased with the gas concentration at lower flow rates, while increased with hydrogen concentration at high flow rates. It was also found that the temperature has a great impact on the morphology of CNT. A very unusual carbon structure, i.e., CNT with beaded carbon, was found. The formation of the unusual carbon structure was discussed.

A13.29 Abstract Withdrawn.

A13.30 EFFECT OF TEMPERATURE GRADIENT NEAR THE TARGET AND GAS FLOW RATE ON THE DIAMETER DISTRIBUTION OF SINGLE-WALLED CARBON NANOTUBES GROWN BY THE LASER ABLATION TECHNIQUE. Rahul Sen, Tokyo Metropolitan Univ. Dept. of Chemistry, Tokyo, JAPAN; Hirochika Katsurada, Tokyo Metropolitan Univ., Dept. of Physics, Tokyo, JAPAN; Yasuake Ohata, Toshihiko Ishigaki, Shinzo Suzuki and Yoshi Aishita, Tokyo Metropolitan Univ., Dept. of Chemistry, Tokyo, JAPAN.

Electronic properties of single-walled carbon nanotubes (SWNTs) depend very crucially on their diameter and chirality. Thus, diameter control during the growth of SWNTs is very important, not only to grow nanotubes having a desired property, but also to understand their growth mechanism. We have studied the effect of temperature gradient near the target and gas flow rate on the diameter distribution of the SWNTs grown by the laser ablation of Ni/Co catalyzed graphite targets. Our results indicate that when the temperature gradient is almost uniform near the target, the gas flow rate has a small effect on the diameter distribution of the SWNTs. However, when the thermal gradient around the target is greater then the gas flow rate affects the diameter distribution strongly. We have also studied the spontaneous emission as well as the scattering images from the laser ablated species at different gas flow rates by using a high speed video camera. We find that the velocities of these species are dependent on the gas flow rate but this dependence is evident only 30-40 m/sec after the laser ablation. Since the gas flow rate affects the final diameter distribution of the SWNTs (especially when there is a large thermal gradient near the target) we can deduce that the growth rates of the SWNTs are much slower than that of fullerene formation.

A13.31 TIME AND SPACE EVOLUTION OF EMITTING CARBON NANO PARTICLES - CORRELATION WITH THE FORMATION OF FULLERENES AND CARBON NANOTUBES. Shinzo Suzuki, Rahul Sen, Hiroshi Yamaguchi, Toshihiko Ishigaki, Yasuake Ohata, Yoshi Aishita, Dept. of Chemistry, Tokyo Metropolitan Univ., Tokyo, JAPAN; Hirochika Katsurada, Dept of Physics, Tokyo Metropolitan Univ, Tokyo, JAPAN.

Time and space evolution of emitting carbon nano particles were investigated using a laser furnace apparatus combined with a high speed video camera or that with an ICCD system. It was confirmed that an apparent increase in the blackbody emission intensity at longer wavelength coincided with the increase in the yield of fullerenes obtained with the same condition. Also, it was found that in our typical experimental condition for making fullerenes and carbon nanotubes, emitting carbon nano particles proceeded in the upstream direction within \( \sim 10 \) m/sec, then spent another a few hundred micro sec inside the furnace, going back to the downstream direction. These findings are used for the discussion on the formation of fullerenes and carbon nanotubes.
MULTIWALL CARBON NANOTUBES AND HOLLOW
NANOPARTICLES BY HYDROTHERMAL TREATMENT.
Jose Calderon-Moreno, Masahiro Yoshimura, Materials and Structures
Laboratory, Tokyo Institute of Technology, Tokyo, JAPAN.

The nanostructure evolution of purified single wall carbon nanotubes
under hydrothermal conditions at temperatures below 800°C and
pressure of 100 MPa, has been studied by high-resolution microscopy
(HRTEM) and selected area electron-diffraction. New layers of rolled
graphite sheets were observed during hydrothermal treatment at this mild
temperature without the presence of any catalyst, resulting in the
formation of multiwall nanotubes and hollow nanoparticles with a
well-defined layered structure, never observed before. In both cases,
the interaction of the rolled graphene sheets with the multiwall nanotubes
formation were found to be hollow multiwall polyhedral nanocages of
concentric bended graphene sheets, with the same graphitic interlayer
spacing. The evolution of this structure and the formation of the multiwall
nanotubes is discussed in the light of the nanostructure evidence.

THE CRYSTALLIZATION OF CARBON NANOFIBRES ON
UNIAXIAL ORIENTED POLYBUTYLENE: 1. G. Bronz, J. Sandler, K.
Schulte, Polymer Composites Section, Technical University
Hamburg-Harburg, Hamburg, GERMANY.

Nano-scale carbon fibres (CNF, supplied by Applied Sciences Inc.,
USA) with a diameter of 10-300 nm, are a new class of material with
the potential to reinforce polymers. The combination of CNF's with
polymer matrices can be considered as a step forward in composites
technology. A fundamental understanding of the CNF / polymer
interaction will further enhance the exchange of materials for high
performance to provide improved semi-crystalline polymers. Ultrathin
films of polybutylene-1 with nanoscale carbon fibres were prepared
either by solution coating techniques or by a special thin film deposition
technique. The dispersion process developed in this project for CNF's
leads to well-separated carbon nanofibers in an uniaxially oriented
crystalline polybutylene-1 film. It is the purpose of this paper to
investigate whether the lattice orientation and spacing of the carbon
nanofibres influence the uniaxially oriented polybutylene-1 matrix.

A THEORETICAL APPROACH TO NANOTUBE FUNC-
TIONALIZATION AND TECHNOLOGY. Thomas Freudenheim
Gotthard Seiffer, Thomas Köhler, Marcus Elstner, Gerd Jungnickel,
University of Paderborn, GERMANY; Efthimios Katsiris, Idzik Park,
Harvard University, MA; Young Ho Lee, Seung-Mi Lee, Jeonseob
National University, Jeonju, KOREA.

We present recent density-functional based investigations on
functionalization of carbon nanotubes (CNT's). Potential problems
and applications of carbon nanotubes are addressed. We focus on
(i) Chemical imaging by interaction of open-end functionalized CNT's with
self-assembled monolayers; (ii) Tailoring of intrinsic electronic
properties for nanoscale electronics by sidewall functionalization of
CNT's with Fluorine; and (iii) Electrochemically based mechanisms
for Hydrogen storage. We further describe in detail the structure,
stability and electronic properties of recently produced
metallic-doped carbon nanotubes. metallic-doped carbon nanotubes,
M$_{x}$B$_{y}$ (M=Mo; Nb) and predict the structure, stability and properties of Silicon- and Silicon-based
tubular structures.

SINGLE WALL NANOTUBE POLYMER FORMS: TYPES AND
MECHANISMS OF POLYMERIZATION, MOLECULAR AND
ELECTRONIC STRUCTURE MODELLING, Leonid A.
Chernozaytseva, Dept. of Macromolecules, Russian Plasma
Physics, Moscow, RUSSIA; Masahiro Momen, Dept of Physics and
Astronomy, Univ Kentucky, Lexington, KY.

We draw attention to a number of high-pressure-high-temperature
structures which retain the SWNT ropes, but in which all the tubes
are connected by means of cycloduction process. We consider
different known for C60 polymers types of the SWNT cycloduction:
(2:2), (2:4), (2:6), (2:8). New monomer fragments, generated during
polymerization bough two crossed (n,m) nanotubes and two parallel
(n,n) and (n,0) SWNT's is discussed. Coupling of two neighbor
nanotubes is energetically favorable under scheme of 'zipper': quick
bind monomeric coupling along two parallel tubes after movement of 2:2
cycloduction of some two atom pairs, disposed one opposite other on
these neighbor nanotubes. Role of hydrogenation in the process of
coupling and depolymerization of SWNT is discussed. The 'zipper'
molecule permits to explain the following: 1) formation of metallic
structures, 2) transformation of molecular coupled nanotube rope
into graphite needle under high pressure treatment, 3) formation of
double diameter nanotubes under high temperature and light atom
flow treatment. 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 crystal structures are computed
by using of molecular mechanics and generalized tight-binding
molecular-dynamic methods; energetic characteristics show high
stability of all these structures; computed energy band structures of
such SWNT polymers show possibility of changing their electronic
properties, from metallic ([12,12] structure) to high dielectric ([6,6]
structure) of porous nanotubes network. The calculations are
supported by the NSF (No. OAR 98-07463) and partially RFII (No.
98-02-1758).

HOTMONE DOPED CARBON NANOTUBES. Bingbing Liu, Jan
Curlsten, Bertil Sundqvist, Dept of Experimental Physics, Umea
University, Umea, SWEDEN.

Carbon nanotubes can be doped by both donors and acceptors, and
in both cases doping leads to charge transfer between dopant and
nanotubes. We present here the results of an experiment in which we
have doped single wall carbon nanotubes, obtained from three
different sources, with bromine. The properties of the doped samples
have been studied using surface enhanced Raman spectroscopy under
ambient conditions and, in one case, under high pressure. In the low
frequency range we observe Raman signals from intercalated bromine
molecules. For large diameter tubes the observed radial breathing
mode frequencies are 10% higher for tubes in bundles than for free
tubes. This result is consistent with theoretical predictions. Doping
also leads to a small shift in the high-frequency modes because of
temperature on. When the doped samples are heated in a vacuum
atmosphere most of the bromine deintercalates from the sample.

INSULATED MOLECULAR WIRE FORMED BY MOLECULAR
NANOTUBE AND CONDUCTING POLYMER. Takeshi Shimomura,
Tomonori Aki, Takashi Abe, Kohzo Iw, Univ of Tokyo, Graduate
School of Frontier Sciences, Tokyo, JAPAN.

Recently, a new series of nanotubes has been synthesized from
acetylenes (n-C6) by Harada et al. This molecular nanotube is soluble
in several kinds of solvents including water and has a small
inside diameter of 0.45nm. Further, this molecular nanotube
include a linear polymer chain with the size matching the inside
cavity of nanotube. In this study, we formed the insulated molecular
wire from the molecular nanotube and a conducting polymer
(polyaniline [PAN]), and observed the conformation of the insulated
molecular wire by atomic force microscopy (AFM). As a result, we
observed the rod-like insulated molecular wires with the length about
300nm clearly by the AFM measurement. This length agrees with the
center length of PAN evaluated from the molecular weight. Further,
the thickness of this molecular is equal to the outside diameter of
the molecular nanotube. In this insulated molecular wire, the nanotubes
show the interaction between conducting polymer chain and
insulating single chain and increase the solubility greatly. In addition, since
the nanotube confines the conformation of the polymer chain to a rodlike
one (all trans configuration) owing to very small cavities, it is possible
that the defects of the conformation system (gauche configuration) are
eliminated from the polymer chain.

SYNTHESIS AND CHARACTERIZATION OF POLYPYRROLE-
CARBON NANOTUBE COMPOSITES. J.H. Chen, W.Z. Li, Z.F.
Ren, Boston College, Department of Physics, Chestnut Hill, MA.

Carbon nanotubes can improve both the strength and conductivity
of organic polymer. Polypyrrole-carbon nanotube composites were
obtained by cycling the potential of a platinum electrode in an
electrolyte solution containing pyrrole monomer and multiwalled carbon
nanotubes suspension. It is observed that the conductivity of the composite
is enhanced by the presence of carbon nanotubes. The composite was...
characterized by cyclic voltammetry, scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

A13.30 CRYSTAL NANOFLUIDS: POLYMER ELECTROLYTES AS NOVEL ACTUATOR MATERIALS. Deljit Sethi, University of Connecticut, Storrs, CT, Ray Nallapeta, Iowa State University, Ames, IA.

Current nanofluidic materials use highly porous, paper-like sheets of nanotubes, which are fabricated with filtration from an aqueous suspension of single-walled carbon nanotubes (SWNTs). This technique yields highly bundled nanotubes, which decreases the effective surface area available for tube layering and also limits the number of nanotubes that can be functionalized. The use of polymeric materials, such as Nafion, allows for high-electrical activation. These composite materials have been shown to exhibit improved mechanical properties (modulus of 2GPa) and strains of about 0.25% in a 25% NaCl solution (vs Ag/AgCl). These composite materials are highly useful for a variety of applications, which is expected to be a useful characteristic for micro-electromechanical systems (MEMS). The effect of the incorporation of these polymeric electrolytes on morphological, area and mechanical properties will be presented.

A13.40 DIAMOND CLUSTERS STRUCTURED WITH NANOFLUIDS:


The emerging field of nanotechnology requires the design of nanoscopic structures that have controllable physical and chemical properties, and that can be constructed from readily available building blocks. Nanodiamonds and carbon nanotubes, for example, are unique structures that can be produced in bulk quantities that have diverse electronic properties depending on their size and morphology. The feasibility of designing configurations composed of nanodiamond clusters and carbon nanotubes as well as their electronic properties will be discussed. Depending on nanotube size and morphology, some types of open nanotubes can be chemically connected with different diamond surfaces, atoms to atoms. For the following nanotube/nanodiamond combinations have been designed: (1,2,0) and (6,0) nanotubes with cubo-octahedral particles, and a (5,5) nanotube with a pentaparticle.

A13.41 STABILITY INVESTIGATION AND THERMAL BEHAVIOR OF MULTI-WALLED CARBON AND SILICON NANOTUBES. Solange B. Faghi, Daniela S. Scorti, Suzana B. Perigotto, Renato Mag. De Fábia, Universidade Federal de Santa Maria, Santa Maria, RS, BRAZIL; R.J. Bierie, Centro Universitário Franciscano, Santa Maria, RS, Brazil, Antonio J.R. da Silva, A. Parizzi, Instituto de Física, Universidade de São Paulo, São Paulo, SP, BRAZIL.

A systematic study about the stability and thermal behavior of multi-walled carbon and silicon nanotubes is presented through two alternative approaches: Monte Carlo simulation using Tersoff empirical potential and first-principles calculations based on density functional theory. Even considering that silicon nanotubes have never been observed and despite the known difficulties for Si in having an sp²-like structure, it is found that both elements have the same valence electron number and a similar distribution of the outermost electrons for the free atoms. As expected, we show that the two nanotubes disintegrate at different temperatures, much smaller for the silicon, reflecting the fact that the sp³ hybridization is more stable in carbon. Also they disintegrate differently, with the Si tend to form more compact 3D-like clusters. At low temperatures, avoiding internal structural deformations, carbon and silicon nanotubes tend to be 1.4 times the GC distance and 1.65 times the Si-Si distance, respectively. In particular, for the double-walled and triple-walled Si nanotubes, we observe that the energy per atom presents a minimum around the temperature where silicon partially recovers its sp³ network. The same behavior is not observed for the carbon nanotubes.


Carbon, silicon and boron-nitride nanostructures were synthesized using microplasma enhanced chemical vapor deposition. Both scanning and transmission electron microscopies were used to observe the morphology and structures while a combination of micro-Raman and electron energy loss spectroscopy were used to determine the composition of the nanostructured materials. Predominantly hollow carbon nanotubes were observed while the Si and BN exhibited a solid, nanoscale structure. All materials were deposited using a thin film iron catalyst seeded on either silicon or boron-nitride substrates with reactive plasma gases containing either methane, ammonia or a mixture of the two. A general discussion of the nucleation and growth mechanisms for the various materials will be included.

A13.43 CARBON NANOTUBE / PMMA COMPOSITES. Sukhoo H. Koo, Bingqin Wei, Linda S. Schadler, Puick Kim A. Joung, Rochester Polytechnic Institute, Dept of Materials Science and Engineering, Troy, NY.

Carbon nanotube based composites, as one of the potential applications of nanotubes, have attracted wide attention in recent years. In this paper, we report the processing and properties of single walled carbon nanotube / poly methyl methacrylate (PMMA) nanocomposites. They were prepared by polymerizing the PMMA in the presence of nanotubes thereby increasing the interaction between nanotubes and PMMA. Tensile tests, DMA, DSC, Raman and four-point probe electrical measurements were employed to characterize the properties of composites. Nanocomposites with 5% carbon nanotubes were found to be electrically conducting. Our results indicate that the interfacing bonding between nanotubes and matrix and resulting mechanical properties depend strongly on the processing conditions. New procedures, involving surfactant-assisted dispersion of nanotubes will be described as a viable route to preparing well-dispersed nanotube composite.

A13.44 HOLLOW FIBERS CONTAINING CARBON NANOFLUIDS FOR STRUCTURAL APPLICATIONS. Carolyn Dry, School of Architecture, University of Illinois, Champaign, IL, Natural Process Design, Champaign, IL.

Filled hollow fibers containing carbon nanotubes and other chemicals have enhanced material strength, electrical, and thermal properties. These issues in nanodiamonds can be controlled by adjusting the physical-chemical properties of the nanomaterials by electron beam erosion and increase device lifetime. Electronic and optical properties of nanostructures consisting of carbon nanoncenes will be also discussed.


We have previously shown that single wall carbon nanotubes (SWNTs) can be filled with C₆₀ molecules by annealing a sample infiltrated with C₆₀ crystals. A C₆₀ vapor is produced, and the fullerene enters the tube via the active site transport or surface diffusion [1]. In this work, we explore the
parameters required to synthesize these C_{60}/SWNT assemblies. The imposition of defects by acid oxidation, the amount of infused C_{60}, and the annealing time and temperature are varied for different samples. Samples are subsequently treated to allow any interior C_{60} that has formed to leach into toluene solution. Each solution is examined using UV-VIS spectroscopy in order to quantify the filling fraction for the corresponding sample. By correlating the measured filling fraction to the varied parameters, we determine the kinetics of the synthesis process, the efficiency of the filling process, and the synthesis condition that maximizes the production of C_{60}/SWNT. The results of this study may enable the bulk synthesis of these so-called bucky peapods, affording the opportunity to measure their properties. The application of our synthesis method for producing hybrid materials using other types of molecules will be discussed. [1]


Pulsed-laser vaporization remains an important research technique for the production of single-walled carbon nanotubes because it allows the greatest amount of control over the nanotube growth conditions, and hence offers the best possibility for gaining control over SWNT structure and morphology. Our work examines structural changes in PLV-grown SWNTs as a function of the growth parameters but especially emphasizes the effects of target composition. Both the catalyst type and concentration are varied and shown to alter the diameter distribution of the resultant nanotubes. An interesting result will also be shown in which the material changes from carbon nanoparticles to "bamboo" structured MWNTs and finally to SWNTs with increased concentration. Nanotube materials are characterized with TEM, Raman spectroscopy, and x-ray diffraction. The results of these will be shown with supporting NMR data, which offers a way to measure the percentages of metallic and semiconducting tubes in a sample.

A13.47 SIMULATING THE IN-PLANE PHOSPHORUS DOPED NANOTUBES. Takuya Higashino, Morinobu Endo, Shintu Univ. Dept of Electrical and Electronic Eng. Nagano, JAPAN.

Doping Boron and Nitrogen into nanotubes has been extensively studied both experimentally and theoretically. The results were interesting in the way that the modification of the electronic properties have occurred, opening possibilities to novel electronic devices. In the world of semiconductors, phosphorus is also playing an interesting role for the effect on the electronic structure. Here, we present the computer simulated results of the phosphorus doped carbon nanotubes. Local structure and electronic properties will be shown.

A13.48 INTERCALATION AND FUNCTIONALIZATION OF CARBON NANOTUBES. Arjun Zhao, Alper Buldum, Jinping Li, Dept. of Physics and Astronomy, University of North Carolina at Chapel Hill; Jie Han, NASA Ames Research Center.

Electronic properties of nanotubes can be dramatically altered with intercalation and chemical functionalization. Using first principles methods we studied the Li intercalation of nanotubes for battery application and functionalization of nanotubes by adsorption of molecules. We find that both the interstitial sites of nanotube rope and the hollow interior of nanotubes are susceptible for Li intercalation. By utilizing both spaces large intercalation depth up to LiC_{60} can be achieved with intercalation potential compatible to Li intercalated graphite. The adsorption of gas molecules, such as O_{2}, N_{2}, H_{2}O, NO, CO_{2}, CO, N_{2}H_{4} and He, has profound impact on electronic properties of nanotubes. The electronic structure calculations show that SWNT can be either charge donor or acceptor depending on the molecule. Thus, the conductive properties of SWNTs can be dramatically changed by exposing to gases, leading to potential application in sensors and devices.

A13.49 ELECTROSPINNING OF CONTINUOUS FIBERS OF CARBON NANOTUBE AND POLYMER COMPOSITE. W. Han, F. Ko, Drexel Uni, Philadelphia, PA; R. Rosen and O. Zhou, Uni. of North Carolina, Chapel Hill, NC.

Electrospinning is an electrostatic induced self-assembly process wherein ultrafine fibers are produced. In this process, a high voltage electric field is generated between an oppositely charged polymer fluid contained in a glass syringe with a capillary tip and a metallic collection screen. As the voltage is increased, the charged polymer solution is attracted to the screen. Once the voltage reaches a critical value, the charge overcomes the surface tension of the suspended polymer with some form of a jet of ultrafine fibers is produced. As the charged fibers are sprayed, the solvent gradually evaporates and the fibers are accumulated on the surface of the collecting screen. This results in a nanoweb mesh of nano to micron scale fibers. We have used the electrospinning method to fabricate fibers of carbon nanotubes and polyethylene oxide using different solvents. Electron microscopy studies show that fibers are continuous and 3 micron in diameter. The structure, morphology and properties of these fibers will be discussed.
A14.2 HYDROGEN STORAGE IN CARBON NANOTUBES: QUANTUM CHEMISTRY AND MOLECULAR SIMULATION STUDIES, B. Jaffe, Songxik Liu, NASA Ames Research Center, Moffett Field, CA.

Recent publications have proposed the use of carbon nanotubes as a hydrogen storage medium. To evaluate the feasibility of these proposals, we have undertaken quantum chemistry and molecular simulation studies to probe the mechanism of hydrogen physisorption and chemisorption in single-wall carbon nanotubes (SWNT) materials. Quantum chemistry calculations are used to determine the interaction energies for the chemisorption of atomic hydrogen and physiosorption of molecular hydrogen on SWNT and graphene surfaces. In this work, sections of the substrates are represented by model clusters with varying curvature and chirality and the effect of electron correlation and basis set incompleteness are included in the calculations. In addition, the possibility of enhancement of the hydrogen-nanotube interaction due to a metal deposition is also studied. Molecular simulation studies include molecular dynamics calculations of molecular hydrogen inside capped nanotubes and interstitial hydrogen storage in SWNT ropes. Modeling of atomic hydrogen migration on curved graphene surfaces is achieved using a semiempirical wavepacket method. The results indicate that neither the curvature of the SWNT surface nor alkali metal doping provides significant enhancement in the binding energy of physisorbed hydrogen. MD simulations at moderate temperatures and pressures reproduce a consistent with < 2 wt% storage capacity for ropes of small diameter SWNT and ~5 wt% for individual nanotubes with diameters of 2 nm.

A14.3 CHARACTERIZATION AND NONLINEAR OPTICAL LIMITING PROPERTIES OF A POLY (ACRYLIC ACID)-SURFACANT-MULTIWALLED CARBON NANOTUBE COMPLEX, Zhanbin Jin, Sun Heng Cai, Guoxiu Xu, National University of Singapore, Dept. of Chemistry, Singapore, SINGAPORE, Lei Huang, Wei Ji, National University of Singapore, Dept. of Physics, Singapore, SINGAPORE.

A poly (acrylic acid) (PAA)-surfactant-multwall carbon nanotube (MWNT) complex was synthesized and characterized using TEM, SEM, XRD, and SAXD. The complex was found to retain a lamellar structure by SAXD, SEM, and TEM. SEM showed that MWNTs were trapped and coated by the lamellar hydrated hemicellulose (C13H16O11) complex. The nanotube trapped inside the complex showed deformable property. TEM micrograph of the PAA-C13H16O11-MWNT complex showed that the nanotube in the complex is nearly 1μm in length with a diameter of 20-30 nm. NLO measurements were made to evaluate the potential application of the PAA-C13H16O11-MWNT complex. Z-scan results showed that the complex showed the same NLO properties as the MWNT suspended in CHCl3. By fitting the standard Z-scan theory, the effective nonlinear refractive index and nonlinear absorption index were found to be about 6.8x10^-18 m^2/W and 4.5x10^-10 m^2/W, respectively. This complex could be a potential candidate for solid NLO devices because of its ease to prepare and film.

A14.4 DEFORMATION ANALYSIS OF SINGLE-WALL CARBON NANOTUBES BY THE VIRTUAL-INTERNAL-BOND (VIB) CONTINUUM THEORY, P. Zhang, Y. Huang, University of Illinois, Dept. of Mechanical Engineering, Urbana, IL; H. Guo, Stanford University, Dept. of Mechanical Engineering, Palo Alto, CA; K. C. Huang, Tsinghua University, Dept. of Engineering Mechanics, Beijing, CHINA.

Carbon nanotubes have exhibited superior mechanical properties over their bulk counterparts. This has attracted significant efforts to study the mechanical behavior of nanotubes, including the deformation pattern and bifurcation mode. These studies, however, have all been limited to the molecular dynamics simulations since the single-wall carbon nanotubes are only a few carbon atoms and are capped at one end. At this level of wall thickness direction, it is commonly believed that the continuum mechanics theories are not applicable at this level. The virtual-internal-bond (VIB) model is a new continuum theory that is capable of capturing the atomic formation into the continuum analysis. We have used the VIB continuum model that builds on theatomic potential of carbon to study the deformation mode of single-wall carbon nanotubes. The predictions of the VIB model agree very well with the molecular dynamics simulations.

A14.5 CARBON NANOTUBES. BUCKYBALLS, ROPES AND A UNIVERSAL GRAPHITIC POTENTIAL L. Girifalco, Miroslav Hrolik and Roland S. Lee, Department of Materials Science, University of Pennsylvania, Philadelphia, PA.

The potential energies of interaction between two parallel, infinitely long carbon nanotubes of the same diameter, and between C60 and a nanotube in various arrangements, were computed by assuming a continuous distribution of atoms on the tube and bulk surfaces and using a Lennard-Jones potential. The total C60-CNT potential is different for graphene-graphene and C60-C60 interactions. From these, the constants for tube-C60 interactions were estimated using averaging rules from the theory of dispersion forces. For tubes in ropes, the cohesive energy per unit length, the compressibility and the equilibrium separation distance were computed as a function of tube radius. For a C60 molecule interacting with tubes, the binding energy inside a tube was much higher than on a tube at the tube mouth. Within a tube, the binding energy was highest at a spherically capped end. The potential energies for tubes of all radii, as well as for interactions between C60 molecules, for a C60 molecule outside of a nanotube, between a C60 molecule and a graphene sheet and between graphene sheets, all fell on the same curve when plotted in terms of certain reduced parameters. Because of this, all the potentials can be represented by a simple analytical form, whereby grafted C60 mimics the computations of van der Waals interactions in graphic system.


We have investigated theoretically transport through metal-carbon-nanotube-metal devices, showing that transport is dominated by length-dependent resonant transmission. Specifically, distinct on- and off-resonance behavior is predicted for armchair tubes commensurate with a 3N, N integer role. Other aspects of resonant tunneling such as peak distributions as a function of nanotube length, helicity and defects will also be discussed. For the case of ferromagnetic leads such as Co, a clear spin-valve effect is predicted for armchair nanotubes with a magnetoresistance ratio of up to 20%. The implications of these results for the fabrications of nanotube devices will be discussed.

A14.7 COMMENSURABILITY AND WETTING PROPERTIES OF KRYPTON ADSORBED ON MULTIWALLED CARBON NANOTUBES: DEPENDENCE ON THE NANOTUBE MORPHOLOGY, D. Bilbaut, A. Boargent, N. Dupont-Paolovsky, J. Galmian, Laboratoire de Chimie du Solide Mineral, Vandoeuvre-les-Nancy, FRANCE; F. Beguin, CH的时间, Lorraine, FRANCE.

Krypton adsorption has been investigated on multiwall carbon nanotubes prepared at the Orleans Laboratory by catalytic decomposition of acetone. The isotherms measured from the first stage of adsorption to the adsorption saturation vapour pressure are compared to those obtained in the same conditions on graphite. The results are discussed in the light of the nanotube morphology, as determined by transmission electron microscopy and electron energy loss spectrometry. Krypton adsorption on the external nanotube walls proceeds, as on graphite, by successive monomolecular layer condensations. The first adsorbed layer is commensurate with the substrate. At its completion, it undergoes a transition towards an incommensurate two-dimensional solid of higher density. The curvature of the graphene sheets, with respect to those of graphite, produces a stabilization of the commensurate film. Moreover, the monolayer condensation pressures are higher than those observed with graphite, which probably limits their number before krypton bulk condensation.

A14.8 DEFECTS ENERGETICS, MECHANICAL INSTABILITY AND LOCALIZED ELECTRONIC STATES IN CARBON NANOTUBES. Roberto Caneschi and Vittorio Reiss, ENEA, High-Performance Computers Project, Centro Ricerche Frascati, and INFN, Rome, ITALY; Fabrizio Cleri, Michael Volpe and Gregorio D’Agostino,
 We report the result of a theoretical study, based on Tight Binding Molecular Dynamics (TBMD), of the thermodynamic properties of different prototypes of carbon and armchair carbon nanotubes. We characterized both the perfect and the defective structures, i.e., in presence of point (vacancies) and topological (5,7 rings) defects. Simulations are carried out at different temperatures up to the onset of the mechanical instability. The origin of such an instability is investigated by means of a topological (order of connectivity). The nanotubes mechanical instability is compared to that observed in other forms of sp²-hybridized carbon structures (e.g. C₆₀). In this latter case, a closed (connected) topological structure unfolds to give origin to disordered graphene sheets. The effect of the different types of defects on the carbon nanotubes physical properties is investigated by evaluating: (a) the change in the instability temperature, (b) the electronic and vibrational density of states, (c) the elastic response. Work performed under the Project “Innovative Materials Based on Carbon Nanostructures” of the Italian Space Agency [ASI].

**A14.10**

**LARGE FIELD EMISSION FROM WELL-ALIGNED CARBON NANOtube AHRAYS.** Jung-Inn Sohn, Seonghoon Lee, Kwangju Institute of Science and Technology, Dept. of MSEK, Kwangju, KOREA; Young-Ho Song, Sung-Yool Choi, Kee-Soo Nam, Micro-Electronics Tech. Labs., ETRI, Taejon, KOREA.

We have grown well-aligned carbon nanotube arrays by thermal chemical vapor deposition at temperatures below 800°C on Fe nanoparticles deposited by a pulsed laser on a porous Si substrate. Porous Si substrates were prepared by the electrochemical etching of p(+100) wafers with resistivities of 3 to 6 Ω cm. These well-aligned carbon nanotube field emitter arrays are suitable for application in micro-emission applications such as cold-cathode flat panel displays and vacuum microelectronic devices like microwave power amplifier tubes. Field emission characterization has been performed on the cold cathode diode device. The mode is maintained at a distance of 60 μm away from the carbon nanotube cathode arrays through an insulating spacer of polyvinyl film. The measured field emitting area is 4.0 x 10⁵ mm². We made a field emission measurement at room temperature. Our carbon nanotube field emitter arrays start to emit 1 mA/cm² at the turn-on electric field, 2 V/μm. Even at 3 V/μm, they emit a large current density as high as 80 mA/cm² which is orders of magnitude higher than any other results reported so far. The field emitter arrays in our diode device are vertically well-aligned carbon nanotubes on the Si wafer substrate.

**A14.11**


A method for distinguishing between metallic and semiconducting single-walled carbon nanotubes (SWNT) in any given sample could be based on the distinct differences in the tangential G-band (≈1500 cm⁻¹) feature in their Raman spectra. The G-band of semiconducting nanotubes has been extensively studied, and is well accounted for using Lorentzian oscillators, and recent polarization studies have identified the symmetries of the various lineshape components. A tailored Bright-Wigner-Fano lineshape analysis of the tangential G-band features attributable to metallic carbon nanotubes is presented. Only two components are needed to account for the entire G-band for metallic nanotubes, both with predominantly A₁g (A₁g) symmetry, and the relative strength of the lineshapes can be used to infer the presence of defects in nanotubes. Surface-enhanced Raman spectroscopy studies show that the coupling mechanism involves the coupling of the G-band tangential phonons (associated with inter-layer deformations) to a surface-plasmon based electronic continuum. Evidence in support of this mechanism is presented, providing a basis for future theoretical calculations.

**A14.12**

**SURROUNDING EFFECTS IN SINGLE-WALLED AND MULTIPLE-WALLED CARBON NANOtubes.** O. Chauvet, Serge Leprat, C. Stehman, J-M. Benoit.

The low frequency Raman observed in SWNT’s has been proved to probe efficiently their diameter distribution. We have made a model to estimate interaction between individual nanotubes when arranged in bundles and shown that an upshift of 6 to 10 cm⁻¹ can be calculated. In a PMMA-SWNT’s composite, our model shows that an upshift can be also predicted, due to the hydrogen bonding applied by the polymer to the bundles. Finally in multilayered carbon nanotubes, the interaction between concentric layers can lead to low frequency modes, as observed experimentally.

**A14.13**

**NNIREAL SHIFT OF SINGLE-WALL CARBON NANOtubes.** Sylvain Lachat, Christophe Gaze, Patrick Bernier, Groupe de Dynamique des Phases Condenses, Montpellier, FRANCE; Luc Henriard, Lab. de Physique des Solides, Namur, BELGIUM; Angel Rubio, Dept de Fisica Teorica, Valladolid, SPAIN.

We report calculation of the NMR chemical shift anisotropy (CSA) tensor of single-wall carbon nanotubes, within the London approximation (ring-currents contribution). Our results clearly indicate that the CSA isotropic line as measured by high-resolution NMR experiments is able to distinguish between metallic and semiconducting tubes (because we predict that the separation of the lines is 11 ppm). We carefully check that this result remains valid and observable when disorder, bends, functionalization and bundle packing are taken into account. Finally, several interesting 3 periods oscillations (magic numbers) in the magnetic response. Packing effect broadening is 20 ppm, but shrink onto a sharp Lorentzian (<1 ppm) when averaging (High resolution NMR).

**A14.14**


Simulations of the diffraction spectra of single-walled carbon nanotubes (SWNT) bundles in the presence of gas are presented in the following cases: i) bundle without gas, ii) tubes filled with gas, iii) gas in the channels between the tubes and iv) gas everywhere in the bundle. We show that the difference curves [empty bundle - gas] are characteristic of each case considered. The measured diffraction patterns of a raw SWNT mat in different environment conditions (in air, in vacuum and after injection of a small amount of water in the sample chamber) are compared to the model predictions. It gives the following results: i) at the beginning of the experiment the air molecules are everywhere in the bundle, ii) after vacuum the water molecules enter preferentially in the tubes core. These results are briefly discussed.

**A14.15**

**MAGNETIC MEMORY OF WELL-ORIENTED CARBON NANOtube FILMS.** Zina Kozlovskaya, Vychodna Kozlovskaya, Yuri Golyev, Alexander Korovin, Yurye Koloskovna, Anna Kozlovskaia, Inst of Radio Engineering and Electronics of RAS, Moscow, RUSSIA.

In our work we studied magnetic properties of well-oriented MoS₂ nanostructures observed in different configurations since the named fullerene like entities to the single and multiple with nanotubes. The corresponding applications are large for the MoS₂ particular characteristics that have been used in typology, catalyt, etc. The High Resolution Electron Microscopy (HREM) techniques have allowed to analyze the structure and local configuration, mainly in the basis of the corresponding contrast. Besides the application of molecular simulation in nanostructure materials has helped a lot in the HREM image interpretation and in the properties prediction or the atomic and electronic distribution involved. This simulation is based in approximation of Molecular Dynamics and Quantum Mechanics theories. In the present work we applied both molecular simulation approaches in order to determine the minimal energy configuration for these structures that implies the geometry optimization for the randomly proposed atomic positions for each one of the models. By using these models we calculated the corresponding HREM image to confirm their existence by comparison with experimental results. Quantum mechanics analysis is also presented to predict the optimal configuration in this kind of materials. Experimental images were obtained from irradiated samples produced by P. Santino in INR for the nanotubes and onion like nanostructured systems facilitated by Prof. Hesleif Tenne.
muli-walled carbon nanotube films on silicon substrates, which were synthesized by electron-beam method [1]. It was shown, that the nanotube films were graphitic nature (the nanotube film was pushed out by magnetic field). Magnetoresistance of nanotube films at different orientation nanotube concerning a direction of magnetic field was investigated. It was obtained, that the magnetoresistance of multiwall nanotube depends on orientation nanotube in magnetic field was changed very much. At the orientations nanotube long and across the direction of a magnetic field the magnetoresistance was negative. But for intermediate orientation of magnetic field the magnetoresistance was sign magnetoresistance. We observed that the nanotube films has the memory to initial magnetic influences. After presence nanotube films in a magnetic field (0.3 T) during long time the magnetoresistance has increase and may achieve the large significance ($\Delta R/R = 0.2$). The relaxation time of magnetoresistance was very big (more than month). Observably anomalous of magnetic behaviour of nanotube films we attribute the one-dimensional character of nanotube structure and the manifestation of quantum effects of the study of magnetic properties of carbon nanotube films is shown the perspective material for sensors magnetic field. This work was supported by grant CRDF #GG-17310-1. Koskovskaya Z.Ya. JETP Lett. 1993, v.56, N1, pp. 2-6.

A14.16
ACOUSTOELECTRON PROPERTIES OF CARBON NANOTUBE FILMS. Georgii Mansef, Sergiej Alekseev, Yuriy Gulyaev, Zoya Koskovskaya, Vladimir Suraikin, Inst of Radio Eng. & Electronics, Moscow, RUSSIA.

Many properties of carbon nanotubes materials were investigated both theoretically and experimentally but the elastic and acoustoelectronic properties of the carbon nanotubes are at the initial stage of the investigation. In this work new methods are used for the experimental study of acoustoelectronic properties of the single-walled carbon nanotube films. The first one is High Overtone BAW Resonator (HBBAR) spectroscopy on microwaves. It was applied to obtain data on material density, sound velocities and the attenuation in the carbon nanotube films. In this series of experiments the influence of the carbon film on resonant peaks frequencies and widths was used as a source of the information. The second method is based on the measurements of SAW propagation characteristics and acoustoelectric effects in layered structures containing the carbon nanotube films. The experiments were carried out using nanotubes synthesized by original method - electron-beam evaporation of pure graphite in vacuum. In HBBAR experiments the carbon nanotube films were evaporated onto the surface of YAG or quartz substrates. The numerical data on mass density, elastic constants and attenuation were obtained. The new previously unknown effect of self-biasing of the nanotubes with time by the elements that are forming the substrate was found an explained. The special investigation in SAW experiments the carbon nanotube films were evaporated onto the surface of yz- LiNbO$_3$. Acoustic attenuation of SAW on 140MHz and acoustoelectric current were observed and the non-linear propagation of transverse magnetic field direction and intensity. The correlation between electric and acoustoelectric phenomena that were observed and some peculiarities of the effect are discussed. This work was supported by grant RFBR #98-02-1730.

A14.17
REINFORCEMENT MECHANISMS IN POLYMER-NANOTUBE COMPOSITES. S.J. Frankland, D.W. Breen, North Carolina State University, Dept Of Materials Science and Engineering, Raleigh, NC, A. Caglar, M. Griebel, University of Bonn, Dept. of Applied Mathematics, Division of Scientific Computing and Numerical Simulation, Bonn, GERMANY.

Carbon nanotubes have been proposed as fillers to mechanically reinforce polymers. The load transfer mechanism between the polymer and nanotube has been investigated with experimental simulation, in model polyethylene matrixes. From molecular dynamics simulation we have estimated that the shear strength of carbon nanotubes in polyethylene is very weak yielding critical lengths (3mm) much longer than is normally physically reasonable for carbon nanotubes. Shear strengths in epoxy matrixes are estimated relative to polyethylene. To allow a more direct examination of the mechanical properties, very large-scale simulations of these composite materials (1.0 micron atoms) will be reported were the modeled carbon nanotube approaches an experimentally comparable size. These simulations implement a parallel version of the Breen potential capable of achieving 0(10$^6$) MD steps per processor, thus allowing the low-mass 512 processes at parallel efficiency of 65% on a CRAY-T3E. A new technique is used to apply tensile stress which varies box shape and size. In addition other reinforcement mechanisms will be considered including the effect of bending the nanotube in the polymer and chemically functionalizing the polymer to the nanotube.

A14.18
APPLICATION OF FLUORINATED CARBON NANOTUBES AND NANOTHERMERS AS AN ENERGY STORAGE MATERIAL. Morimatsu Endo, Takuya Hayashi, Y.A. Kim, Shinshu Univ, Dept of Electrical and Electronic Eng., Nagano, JAPAN.

Carbon nanotubes and nanothermers are promising as a electrode material for the Li-ion batteries and capacitors. The market demands for a higher storage capacity because the mobile information technology devices are so widespread and people ask for a longer battery life for such devices have been observed. The high energy storage capacity, and carbon nanotubes and nanothermers survived the competition. In the past, we have showed that hor-boron-doped nanotubes and fibers' energy storage capacity is very high. In this paper we report the high performance hor-boron-doped nanotubes and fibers which is different from the non-doped fibers. In the present work, according to the knowledge that we have obtained in the previous studies, microstructure study using energy-filtered transmission electron microscopy and Raman spectroscopy and application of the fluorinated carbon nanotubes and nanothermers as an energy storage materials will be shown. Obtained results will be compared with the microstructure and energy storage capacity of boron-doped nanotubes.

A14.19
PRESSURE DEPENDENCE OF THE RAMAN MODES IN IODINE DOPED SINGLE WALL CARBON NANOTUBE BUNDLES. Umar D. Venkateswaran, E.A. Brodskien, Department of Physics, Oakland University, Rochester, MI, A. Harutyunyan and P.C. Eklund, Department of Physics, Pennsylvania State University, State College, PA.

Successful doping of single wall carbon nanotube (SWNT) bundles with iodine molecule has been shown to produce a charge transfer compound which is a stable superconducting compound [1]. The Raman spectrum of the iodine doped SWNT (I-SWNT) contains the radial breathing (R) and tangential (T) vibrational modes of SWNT as well as modes due to polycrystalline iodine [1]. In this paper we report the pressure dependence of the I$_{2}$ SWNT. With the 514.5 nm excitation, the strongly resonant (I$_{2}$) mode, which is at 179 cm$^{-1}$ at ambient pressure, softens gradually by about 3 cm$^{-1}$ until 3 GPa and then gradually hardens by the same amount up to 5.5 GPa. This pressure-induced shift is very weak compared to the shift of the 514.5 nm /GPa compared to the T-modes in the same pressure run and also as reported earlier for the T-modes in undoped SWNT [2]. The intensity of the (I$_{2}$) mode is found to decrease smoothly with increasing pressure. The ratio, S, of the peak intensity of the (I$_{2}$) mode to that of the T-modes, shows an initial increase, an abrupt increase near 2 GPa, and then remains more or less a constant between 2 and 5.5 GPa. The discontinuity in S is due to an abrupt decrease in the T (and R) mode intensity at 2 GPa, which has been attributed to a geometrical distortion in the cross-section of the SWNT bundle [2]. The weak pressure shift of the (I$_{2}$) mode observed in this study, is consistent with the recently reported zero-charge transmission electron microscopy images showing that the polycrystalline iodine resides inside the SWNTs [3] [1]. B. Grigoriev et al., Phys. Rev. Lett. 80, 5560 (1998), [2] U.D. Venkateswaran et al., Phys. Rev. B 59, 10 928 (1999), [3] X. Fan et al., Phys. Rev. Lett. 84, 4621 (2000).

A14.20
EFFECT OF GAS ADSORPTION AND COLLISIONS ON TRANSPORT PROPERTIES OF SWNTS. G.L. Sumashekara, C. Adu, K.A. Williams, P.C. Eklund, Department of Physics, Pennsylvania State University, University Park, PA.

The effects of gas adsorption and collisions on the thermolectric power and resistivity of tangled bundles of single-walled carbon nanotubes (SWNTs) are investigated. Degassing samples in vacuum at 500 K drives the thermo-power strongly negative, indicating that the degassed metallic tubes in a homogenous gas environment approach an experimentally comparable size. These simulations implement a parallel version of the Breen potential capable of achieving 0(10$^6$) MD steps per processor, thus allowing the low-mass 512 processes at parallel efficiency of 65% on a CRAY-T3E. A new technique is used to apply tensile stress which varies box shape and size. In addition other reinforcement mechanisms will be considered including the effect of bending the nanotube in the polymer and chemically functionalizing the polymer to the nanotube.

A14.21
EFFECT OF GAS ADSORPTION ON TRANSPORT PROPERTIES OF SWNTS. C. Adu, G. Sumashekara, P.C. Eklund, Department of Physics, Pennsylvania State University, University Park, PA.

The effects of gas adsorption and collisions on the thermolectric power and resistivity of tangled bundles of single-walled carbon nanotubes (SWNTs) are investigated. Degassing samples in vacuum at 500 K drives the thermo-power strongly negative, indicating that the degassed metallic tubes in a homogenous gas environment approach an experimentally comparable size. These simulations implement a parallel version of the Breen potential capable of achieving 0(10$^6$) MD steps per processor, thus allowing the low-mass 512 processes at parallel efficiency of 65% on a CRAY-T3E. A new technique is used to apply tensile stress which varies box shape and size. In addition other reinforcement mechanisms will be considered including the effect of bending the nanotube in the polymer and chemically functionalizing the polymer to the nanotube.
The effects of H$_2$, NH$_3$, and H$_2$O adsorption on the thermoelectric power (TEP) and resistivity of single bundles of single-walled carbon nanotubes (SWNTs) are investigated. Degassing samples in vacuum at 500 K drives the thermopower strongly negative, indicating that the degassed metallic tubes in a bundle are n-type. By a systematic study of TEP and resistivity of degassed SWNTs when exposed to oxygen at 500 K with varying partial pressure, we found that for smaller partial pressures ($P < 10^5$ Torr) TEP becomes positive with increasing resistance in a reversible manner. But for larger partial pressures ($P > 10^5$ Torr), the TEP becomes strongly positive and in sharp contrast to the $P < 10$ Torr results, the resistance decreases. Adhesion of H$_2$ and NH$_3$ drives the thermopower further negative (less negative), the values obtained from "degassed" tubes while the resistivity is still increasing. For H$_2$, adsorption/desorption is fully reversible, but only partially reversible for NH$_3$. Results of H$_2$ partial pressure dependence on electrical transport properties at 500 K, 300 K and 77 K are also presented. This work was supported by Grant NSD 98-10986 and DOD DAA07-97-C-J095.

A14.22 FIRST-PRINCIPLES CALCULATIONS OF IODINE ATOMS INSIDE SINGLE-WALLED CARBON NANOTUBES
SangYool Cho, Kee Soo Nam, KyungIl Cho, Micro-Electronics Technology Laboratory, ETRI, Taejon, SOUTH KOREA.

Recent experiments and calculations by Grigorian et al. [Phys. Rev. Lett. 80, 5560 (1998)] and Fan et al. [Phys. Rev. Lett. 84, 4621 (2000)] show that iodine atoms inside single-walled carbon nanotubes arrange in the form of helical chains and increase prominently electrical conductivity by orders of magnitude, but the structure and properties are not completely explained. In this work we investigate structural and electronic properties of iodine-intercalated single-walled carbon nanotubes and explore the effect of charge transfer on the physical properties of these novel systems from first-principles calculations. Our calculations are based on the density functional method with local density approximation of exchange-correlation functionals, norm-conserving pseudopotentials and supercells.

A14.23 TRANSFERRED TO A12.3

A14.24 COMPRESSIBILITY OF FULLERENEFILLED CARBON NANOTUBES
Jie Tang,1 LuChang Qin,2 Shanjil Bandow2 Masako Yashima2, Tatsuo Sasaki1, Akira Yamasaki1 and Sumio Iijima1,3,4,5
1National Research Institute for Metals, Tsukuba, JAPAN; 23ST Nanotube Project, c/o NEC Corp., Tsukuba, JAPAN; 3Japan Nanotube Project, c/o Mejo Univ., Nagoya, JAPAN; 4R&D Group, NEC Corporation, Tsukuba, JAPAN; 5Dept. of Mat. Sci. & Engg., Mejo Univ., Nagoya, JAPAN.

Though carbon nanotubes are very strong in their axial direction with an intrinsic Young's modulus, they are soft in the radial direction due to the hollow core. When such carbon nanotubes are filled with fullerenes to form the peapod structures, it is expected that their radial modulus will be increased. We have carried out a measurement of the radial compressibility of several peapod structures using a diamond-tipped press cell combined with in situ synchrotron X-ray diffraction. It is shown that the radial stiffness of the C60 fullerenefilled carbon nanotubes has been greatly strengthened compared with the unfilled nanotubes. The volume compressibility of the C60 fullerenefilled peapod nanotubes has been reduced by about 30% from the unfilled starting single-walled carbon nanotubes. Details and implications will also be presented and discussed.

A14.25 EXTRACTION OF CARBON NANOTUBES BY AN AFM TIP
Sailing Zoucha1,2,4,10,11, Jegor Fedorov1,2,4,10,11, Giovanni Cappello3,4,10,11, Guillaume Pouget3,4,10,11, Marie Bourbon3,4,10,11, Iris Sinigir6,1,2,4,10,11, Jürgen Schüller6,1,2,4,10,11, Institut Curie, Laboratoire Physico-Chimie-Christie-Curie, Paris, FRANCE; 3LÉPES-CNRS, Grenoble, FRANCE; 4Université Joseph Fourier, Grenoble, FRANCE.

Micrometer thick layers of multivall carbon nanotubes (nanotube carpet) have been produced by Hot Filament Chemical Vapor Deposition. Atom Force Microscopy (AFM) in the phase detection mode and Scanning Electron Microscopy reveal that the nanotubes, typically 20 nanometers in diameter and more than 1 micrometer long, are entangled. AFM force-distance curves are used to investigate the interaction of the AFM tip with the nanotube carpet. This provides information on the adhesive properties between the nanotubes and the silicon nitride tip and on the deformation properties of this nanotube carpet. If the AFM tip is strongly pressed against the layer, force-distance curves clearly reveal that many nanotubes are interacting with the AFM tip. In the case of a soft contact, we demonstrate that just a few nanotubes interact with the tip (prismatically down to a single nanotube). A low force microcantilever is observed in force curves. This is an evidence for a non-linear response of the contacted nanotubes due to both their bending and stretching. A simple numerical simulation based on the Van der Waals interaction between a set of nanotubes and the AFM tip reproduces the experimental characteristic features of the adhesion and the friction. Transport of nanotubes extracted from the nanotube carpet using the AFM tip, their deposition onto a clean silicon wafer and their characterization with AFM motivate in friction mode with a clean tip are also demonstrated.

A14.26 ABSTRACT WITHDRAWN

A14.27 MOLECULAR MECHANICS OF BINDING IN CARBON NANOTUBE-POLYMER COMPOSITES
Vincenzo Lordi, Nan Yao, Princeton University, Princeton, NJ.

Nanoscale composites have been a technological dream for many years. Recently, increased interest has arisen in using carbon nanotubes as filler for polymer composites, owing to their very small diameters on the order of 1 nm, very high aspect ratios of 1000 or more, and exceptional strength with Young's modulus of ~1 TPa. A key issue for realizing these composites is obtaining good interfacial adhesion between the phases. In this work, we use force-field based molecular mechanics calculations to determine binding energies and show that frictional stresses between pristine carbon nanotubes and a range of polymer substrates, in an effort to understand the factors governing interfacial adhesion. The particular polymers studied were chosen to correspond to reported composites in the literature. We also examined polymer morphology by performing energy-minimizations in vacuum. Hydrogen bond interactions with the polymer of pristine carbon nanotubes are found to bond most strongly to the surface, in the absence of chemically altered nanotubes. Surprisingly, we find that binding energies and frictional forces play only a minor role in determining the strength of the interface, but that helical polymer conformations are essential.

A14.28 SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY OF MULTIVALL WALL CARBON NANOTUBES
Abdol Hosseini, Motoko Takeuchi, Electrotechnical Laboratory, Tsukuba, Ibaraki, JAPAN; X. Zhao, and Y. Ando, Department of Physics, Meijo University, Shiogamaguchi, Tempaku-ku, Nagoya, JAPAN.

We report on the structural analysis of multivall wall carbon nanotubes (MWNNTs), produced by DC arc discharge in hydrogen gas, using a scanning tunneling microscope operated at ambient conditions. On a microscopic scale the images show tubes condensed in ropes as well as individual tubes which are separated from each other. Individual nanotubes exhibit various diameters (2-6 nm) and chiralities (0,30). For MWNNTs, the outer diameter is composed of highly oriented nanotubes with nearly uniform diameter (4.5 nm) and chirality. Strong correlation is found between the structural parameters and the electronic properties in which the MWNNTs span the metallic-semiconductor regime. True atomic-resolution topographic STM images of the outer shell show hexagonal arrangements of carbon atoms that are equally visible by STM top. This suggests that the stacking nature of MWNNTs has no detectable effects on the electronic band structure of the tube shell. Unlike other MWNNTs produced by arc discharge in helium gas, the length of the tubes are rather short (80-500 nm), which make it feasible to use them as a components for molecular electronic devices.

A14.29 TENSION AND BENDING OF CARBON NANOTUBES
Laszlo Vecsei,1 Christophe Goze, Patrick Bernier, GCDP, UMR 5581, MontpellierT H Univ, Montpellier, FRANCE; Angel Rubio, DPT, Valladolid Univ, Valladolid, SPAIN.

We report on a theoretical investigation of the elastic properties of single walled carbon nanotubes. The nanotube response is examined under axial, torsional and bending strains using a non-orthogonal tight binding method. The Young's modulus, Poisson ratio, torsional and bending moduli were calculated for several nanotubes with various diameters and chiralities. The results demonstrate that single walled carbon nanotubes are both extremely stiff in the axial direction and flexible. The torsional and bending moduli are almost insensitive to the helicity of the tube but depend strongly on its diameter. These moduli are also estimated with the continuum theory of elasticity and compared to the available experimental values.

A14.30 NANOMANIPULATION AS A PATHWAY TO NANOTUBE-BASED
Carbon nanotubes are promising materials for nanoscaled devices due to their unique electrical and mechanical properties. Nanobeaded devices need specific configurations of nanotubes. Using the tip of an atomic force microscope (AFM) as a manipulation tool one can overcome the problem of the randomly distributed arrangement of nanotubes on a substrate. In this context, an AFM tip layout of nanotubes is created. Here we demonstrate how a commercial AFM without any technical changes can be used for this purpose. We developed a protocol which allows us to perform multistep manipulation of single-walled nanotubes (SWNTs) or SWNT bundles in a reliable and controlled manner. Simultaneous measurements of the normal and lateral forces during the manipulation give us insight into the mechanism of the nanoscaled movement of objects (bending, sliding, unswelling of bundles).


The crystal growth behavior and crystallography of a variety of metal halides incorporated within single-walled carbon nanotubes (SWNTs) as determined by high resolution electron microscopy (HREM) is described. Single-packed structures, such as the niobium halides form enriched structures within SWNTs that are integral atomic layers in terms of their thickness. An enhanced HREM image restoration technique reveals precise detail concerning lattice distortions present in these crystals. More complex structures formed within SWNTs, such as those derived from 3D complex, layered and chain halides form related crystal structures within SWNTs. In narrow (i.e. > 1nm diameter) SWNTs, these halide framework structures that consist of individual 1D polyhedral chains (1D-PHG) derived from the corresponding bulk halides within SWNTs. In the case of the 3D complex and layered halide structures, the polyhedral chains form with lower co-ordination than in the bulk. Molecular halides also form within SWNTs, but these are frequently disordered and do not readily form ordered structures within SWNTs.

14.3.2 MICRO-RAMAN INVESTIGATION OF ALIGNED SINGLE-WALL CARBON NANOTUBES. M.A. Pimenta, C.F. Leite, M.S. Sattam, UFV-UFMG, Belo Horizonte, BRAZIL; D. Ugarte, LNLS, Campinas, BRAZIL; H.M. Cheng, Institute of Metal Research, Shenyang, CHINA; K. Kajimura, A. Link; University of Kentucky, Lexington, KY; A. Jorio, G. Dresselhaus, M.S. Dresselhaus, MIT, Cambridge, MA

Aligned single-wall carbon nanotubes (SWNTs) were prepared using the hydrogentransfer and arc-discharge method, and the samples exhibit a good nanoscale alignment. Polarized micro-Raman experiments, allowing a spatial resolution of 1µm, were performed in samples prepared in special substrates and previously characterized by TEM. Using degenerate and non-degenerate lines, we observed the Raman signature from the sample exhibits diameters in the range of 1.15 ± 0.25 µm, giving rise to a broad band in the Raman spectra around 120 cm⁻¹, associated with the radial breathing mode (RBM) of the tubes. However, very sharp Raman peaks are sometimes found superimposed on the broad RBM band, indicating also the presence of small diameter SWNTs in the sample. The frequencies of these sharp peaks depend on the position of the laser spot on the sample, revealing the presence of isolated small diameter SWNTs or SWNTs of the same diameter, but with different shapes of the tangential band, between 1500 and 1600 cm⁻¹, when the position of the laser beam changes from spot to spot on the sample, and by comparing the Raman shifts of the RBM and tangential bands, it is possible to differentiate the Raman spectrum coming from isolated semiconducting and metallic SWNTs.

14.3.3 ELECTRONIC AND STRUCTURAL PROPERTIES OF METAL-SEMICONDUCTING JUNCTIONS IN CARBON NANOTUBES. S.P. Machado, P. Piquini, R. Meier Depto. de Física, Universidade Federal de São Paulo, São Paulo, RS, BRAZIL; R. Fucini, Instituto de Física, Universidade de São Paulo, São Paulo, SP, BRAZIL.

The electronic and structural properties at the Fermi level of junctions produced by connecting two or more nanotubes with different helicities are investigated using two different approaches. The first is based on Monte Carlo simulation with empirical Tight Binding potential and the second is an electronic calculation through self-consistent field Hartree-Fock-Roothan method. One main target of this work is to find a (10,0)/(6,6) junction which connects a semiconductor tube with a metallic one by introduction of a pentagon-heptagon pair defects diametrically opposed in the structure. In this case, the optimized structure implies in a kink that forms an angle of approximately 36° on the junction between the two tubes. In particular, we have assumed previously optimized structures using a simplified molecular mechanics model. Using an empirical Tight Binding potential we discuss the energy gain of the junction and the corresponding Fermi level. The basis for HOMO and the lowest unoccupied molecular orbital (LUMO) are determined for the (10,0) and (6,6) nanotubes and for the junction. For the pure (10,0) and (6,6) nanotubes, the σ is the dominant character for both HOMOs. The local electronic states of the metallic-semiconducting junction region present a mixture of characters and the corresponding LUMO of HOMO is displaced for the semiconducting region, creating the condition for electronic localization devices at the nanometer scale. We also determine how these properties change from the metallic to semiconducting side of a nanotube junction. Also, preliminary results for the semiconducting-metallic-semiconducting ((10,0)/(6,6)/(10,0)) heterojunction permit the discussion about the properties of the associated single-electron transistor.

14.3.4 PROGRESS ON CNT NANOELECTRICAL/MECHEANICAL DEVICES. Phillip Williams, Neal Snyder, Scott Paulson, Michael R. Falvo, Sean Washburn, Richard Superfine; The University of North Carolina, Dept. of Physics and Astronomy, Chapel Hill, NC.

Using e-beam lithographic techniques, substrate etching, and AFM manipulation, we have created a variety of integrated nanotube device structures that include suspended and cantilevered tubes, and CNT/CNT contacts. In a system directly relevant to CNT/CNT contacts, we have found that the resistance of the CNT/HOPG contact depends on the relative angle of the contacting graphene lattices and have also explored the locality of these circumferential transport modes. We have manipulated CNT/CNT contacts through AFM or electron photodarkening in order to probe the effect of relative lattice translation and rotational orientation on contact resistance. Progress on an integrated electromagnetic resonator, CNT/CNT transport measurements, and atomic scale effects of tubes-on-tube contacts will be presented. This work was supported by the National Science Foundation (DPC8, ECS), the Office of Naval Research (MURI), and National Institutes of Health (NCRR).

14.3.5 ELECTRONIC BAND STRUCTURE STUDY ON CARBON NANOTUBES USING ANGLE RESOLVED ULTRAVIOLET AND X-RAY PHOTOEMISSION SPECTROSCOPY. Jiawen Chei, Louisiana State University for Advanced Computing and Devices, Baton Rouge, LA; Young Lee, Jeonbuk National University, Jeonju, KOREA; Hyeong Seok Yoo, Exxon Mobil Process Research, Baton Rouge, LA.

Electronic band structure of the vertically aligned multiwall carbon nanotubes has been experimentally studied using angle resolved ultraviolet photoemission spectroscopy and core level photoemission spectroscopy. The finite thicknesses of layers near the Fermi level were observed. The valence band dispersion of the multiwall carbon nanotubes was small unlike the calculated band dispersion of the single wall carbon nanotube. There are two main peaks which are at 3.05 eV and 7.66 eV. These valence band structures indicates the electronic structure of the multiwall carbon nanotubes is more like the electronic structure of the polycrystalline graphite than fullerenes. The carbon is core level spectra support that there are strong SP2 hybridization character for SPS character. By changing the amount of Ar ion sputtering, the electronic structure of the carbon nanotubes resembles to the amorphous carbon.

14.3.6 ABSORPTION OF HYDROGEN ON CARBON SINGLE WALL CARBON NANOTUBES AS MEASURED BY THE VOLUMETRIC TECHNIQUE. Philip A. Parilla, Anne C. Dillon, Jeffery L. Allman, Kim M. Jones, and Michael J. Heben, National Renewable Energy Laboratory, Golden CO; Thomas Germer, Department of Chemistry and Center for Materials Science, Rochester Institute of Technology, Rochester, NY.

Of the many possible applications for carbon single-walled nanotubes (SWNTs), one of the most intriguing is for the storage of hydrogen. As previously reported, [1] hydrogen absorption onto single-walled carbon nanotubes (SWNTs) has given storage density of 19.5 wt% and this is estimated between 5 and 10 wt %. This would provide high energy
storage efficiencies for applications requiring lightweight storage capabilities such as for vehicles. Since this original report, much effort has been aimed at developing the growth and purification of SWNTs as well as understanding the nature of their hydrogen absorption. This has resulted in highly pure samples capable of absorbing up to ~7 wt % hydrogen as measured by temperature programmed desorption (TPD). While we have gone to great efforts to ensure that the calibration of the TPD results are accurate, it is important to verify these exciting results using another measurement technique. Here, we report on hydrogen absorption onto SWNTs as measured by the volumetric technique. This method determines the amount absorbed by monitoring the pressure in a known volume at a known temperature with a given number of moles of hydrogen introduced. The raw material for the samples produced through pulsed laser vaporization of a graphite target containing Ni (0.6 at %) and Co (0.6 at %) dopants is followed by a purification procedure and then by a cutting procedure. Finally, the sample is degassed before the hydrogen absorption is measured. A description of the apparatus used to determine the tubular surface area by the B E T technique will be presented.

A14.37 TOPOLOGY AND ENERGETICS OF THE MECHANICALLY SIGNIFICANT DEFECTS IN BN NANOTUBES. H.F. Bettinger 1,2, G.E. Scuseria 1,2, and J.I. Yudson 1,2.

The alternating chemical order in the boron nitride lattice makes the atomic relaxation mechanism different than in a similar hexagonal carbon lattice. We calculate the topology and energetics of the defects responsible for the mechanical relaxation and strength of BN nanotubes. In this work, we explore the semiempirical AM1 Hamiltonian and density functional theory in combination with the polarized all-electron 6-31G(d) basis set. The analogue of the Stone-Wales transformation in BN produces a dislocation dipole of \( b_1 \), represented by a 5/7/7/7 ring defect containing B-B and N-N bonds. It corresponds to a local potential energy minima and is thus metastable. Another important defect with the presence of an alternating B-N bonding pattern is proposed, a 4/8/8/4 dipole of Burgers vector \( b = \frac{1}{2}(1,2) \). Whereas for the free defects in nanotubes, both alternatives are similar in energy, the B-B-N-N structures are significantly more favorable energetically by \(-4.4 \text{ eV} \) for the dipole incorporated into a finite unstrained BN tube or sheet. The comparison with the analogous all-carbon structures indicates that the formation of the 5/7/7/7 defect requires more energy for BN nanotubes.

A14.38 PROPERTIES OF GAS ADSORPTION ON SINGLE WALL CARBON NANOTUBES. Hiromori Ogata, Institute for Molecular Science, Okazaki, JAPAN, Syogo Kuno, Yakushi Sato, Dept. of Electrical and Electronic Engineering, Me University, Tsu, JAPAN.

We present the results of the N2, O2, and several kinds of inert gas adsorption isotherm of both end-capped and end-opened single wall carbon nanotubes (SWNTs). The samples used in this study were synthesized by the dc arc discharge method using Pt-Rh mixed catalyst. Amorphous carbon contained in the raw soots were removed by using hydrogen peroxide (H2O2). The end-opened samples were synthesized by doing appropriate heat treatment in air. The \( \alpha \)-plot analysis of N2 adsorption isotherms at 77K revealed that heat treatment increase the intensity of two upward swings (filling- and condensation-swing) below \( a = 1.0 \). This fact suggest that the heat treatment lead to the micro pore filling and capillary-like condensation inside the tube space. Analysis of the other gas adsorptions will be discussed in this presentation.

A14.39 EVIDENCE FOR LUTTINGER LIQUID BEHAVIOR IN MULTI-WALLED CARBON NANOTUBES. E. Gruneis, R. Reidenberger, Purdue Univ, Dept of Physics, W. Lafayette, IN, B. Kiehl, A.W. Ghosh, S. Dotz, Purdue Univ, Dept of Electrical and Computer Engineering, W. Lafayette, IN, P.J. de Pablo, Universidad Autonoma de Madrid, Dept. Fisica de la Materia Condensada, Madrid, SPAIN.

We report on the conduction of multiwalled carbon nanotubes as a function of voltage and temperature between room temperature and 4.2K. The data show a monotonic decrease in conductance as the temperature is lowered. At temperatures below ~20K, a non-linearity develops in the V(I) data, corresponding to a pronounced dip in the conductance near zero bias. The size of the dip increases as the temperature is lowered. The data are explained in terms of the Luttinger liquid model for transport.

A14.40 PROPERTIES OF XENON GAS ADSORBED INSIDE SINGLE WALL CARBON NANOTUBES. Hiromori Ogata, Institute for Molecular Science, Okazaki, JAPAN, Syogo Kuno, Yakushi Sato; Dept of Electrical and Electronic Engineering, Me University, Tsu, JAPAN.

Pressure and temperature dependences of 129Xe-NMR were performed by xenon gas adsorbed single wall carbon nanotubes produced using non-ferromagnetic Rh-Pt mixed catalysts by arc discharge method. Appropriate heat treatment was proved to be essential to open the tubules and cause Xenon gas adsorption inside the single wall carbon nanotubes. Detailed dynamics and thermodynamic properties of Xe-NMR measurements obtained by adsorption isotherm and NMR measurements will be discussed.

A14.41 EFFECT OF ORGANIC POLYMER SOLUTION IN PURIFICATION AND CUTTING OF SINGLE-WALL CARBON NANOTUBES. Manako Yudohi, Masatake Zhang, Christopher Jobs, and Samio Iijima, Tohoku University, JAPAN, Meijo University, Dept. of Physics, Nagoya, JAPAN.

Single-wall carbon nanotubes (SWNTs) formed by laser ablation and arc discharge contain various impurities which include amorphous carbon, metal catalysis, and graphite particles. It has been shown that oxidation using acids such as nitric acid helps to remove these impurities. Mizoguchi et al. has also suggested the use of ultra fine gold particles to catalyze the oxidation of amorphous carbon at lower temperatures[6]. Purification using strong acids has shown to generate shortened tubes, whose properties have been characterized by various analyses methods, such as scanning tunneling microscope. However, we think that purification using acids may cause safety and environmental problems if they were employed in large scale production of SWNT in future. We have been searching for an alternative purification method that would not require the use of strong acids, and here we found that a polymer solution is helpful to purify and shorten SWNTs. This method also facilitates the isolation of single SWNTs by allowing us to disperse the tubes on a substrate by spin coating. [1] E. Mizoguchi et al. Chem. Phys. Lett. 321 (2000) 297.

A14.42 HYDROGEN STORAGE IN CARBON NANOTUBES. Andrea Quante, Youngmoon Choi, Ursula Deflath, Viera Skalakova and Sigmund Rieh, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, GERMANY, Michael Becker, Miro Hulka and Michael Hirsch, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY; Raimund Strobel and Ludwig Joeris, Zentrum fuer Solarenergie und Wasserstoffforschung, Ulm, GERMANY.


SESSION A15 NANORODS/TUBES

Chair: Otto Zhou

Thursday Morning, November 30, 2000

Grand Ballroom (Sheraton)

8:30 AM *A15.1 OXIDE-ASEMITYED SYNTHESIS OF ONE-DIMENSIONAL SEMICONDUCTOR NANO-MATERIALS. S.F. Lee, Center of Super-Diamond and Advanced Films (COSDAF) & Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, SAR, CHINA.

Our recent studies have shown that by using oxides as a starting material in a laser ablation, thermal evaporation or CVD process, it is possible to achieve bulk quantity synthesis of high-purity [no metal contamination] one-dimensional nanoscale semiconductor materials.
9:00 AM A15.2 SYNTHESIS AND CHARACTERIZATION OF SELENIUM NANOWIRES WITH UNIFORM, WELL-CONTROLLED DIMENSIONS: Byron Gates, Xuying Dong, Younan Xia, Univ. of Washington, Dept. of Chemistry, Seattle, WA.

We have recently demonstrated an effective chemical approach to the large-scale synthesis of single crystalline selenium nanowires with uniform, well-controlled linear dimensions in the range of 10-100 nm. In this talk, we will discuss the mechanism for the formation of these single-crystalline, anisotropic nanostructures versus zero-dimensional, isotropic colloidal particles. The unique optical and photoelectrical properties of these nanowires will also be presented.

9:15 AM A15.3 CATALYST-FREE SYNTHESIS OF SINGLE-WALLED BORON NITRIDE NANOTUBES VIA LASER ABLATION: Baland S. Lee, Julie Guillet, Marc Lamy de la Chapelle, Annick Lequesne, LEM, CNRS ONERA (UMR704), Château Cedex, FRANCE; Jian-Lou Cochon, Daniel Pipache, ONERA, Palais des Cedex, FRANCE; Tatsin Thilmans, SP3M, DRFMC, CEPI, 85X, Grenoble Cedex, FRANCE; Francois Tailleb, SARC, CEA Saclay, Gif-sur-Yvette Cedex, FRANCE.

We present the results of catalyst-free synthesis of boron nitride nanotubes (BN-NWs) in ‘nanotubes’ quantities (~150 mg) using a continuous CO2 laser ablation reactor described in the literature [1]. High-resolution transmission electron microscopy (HRTEM) analyses have shown that the samples are composed of single-wall boron nitride nanotubes (BN-SWNTs) in long (~100 nm) perfectly crystallized ropes (~5-10 nm in diameter). The samples also contain a small percentage of BN-NWs synthesized using a method of plasma-activated vacuum filtration of BN-SWNTs. Using fast Fourier Transform to obtain their densities, the majority of BN-SWNTs organized in ‘ropes’ seems to have a zigzag configuration. The BN-NWs also appear to grow from the surface of the BN-SWNTs, and the growth rate was determined using electron emission loss spectroscopy (EELS). These results are particularly interesting as they represent the first time that BN-NWs have been synthesized in quantities and quality comparable to that of carbon nanotubes. The advantage that no catalyst was needed. Since bulk production of this material has now been realized, its characterization, using methods previously studied by the group, is now possible [2].

9:30 AM A15.5 STRESS-INDUCED MECHANICAL PROPERTIES OF SILICON CARBIDE-BASED MATERIALS: Z.R. Dai, Z.G. Bu, R.P. Gao, Z.L. Wang, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA; J.L. Gele, J.D. Stout, School of Physics, Georgia Institute of Technology, Atlanta, GA.

One-dimensional carbon nanotubes are of fundamental importance to the study of size-dependent physical and chemical phenomena. With a relatively high mechanical strength and chemical inertness, carbon nanotubes have found applications in optoelectronics, nanomechanics, and nanoelectronics. The mechanical properties of carbon nanotubes are an important factor in determining their applications in these fields. In this work, we present the stress-induced mechanical properties of silicon carbide-bonded silicon carbide nanowires. The stress-induced mechanical properties of silicon carbide nanowires are important for understanding the behavior of these nanowires under various conditions. The stress-induced mechanical properties of silicon carbide nanowires are determined using a combination of experimental techniques, including in situ mechanical testing and density functional theory calculations. The results of these experiments provide important insights into the behavior of silicon carbide-based nanowires under stress conditions.
as effective 1-D substrates for high signal-noise studies of single molecules and atoms over a wide temperature range.

11:00 AM A16.2 


In a rare occasion a SWNT could trap fullerenes in its central hollow during laser ablation of graphite [1], which is so called “peapod” [2]. The observation motivated us to make SWNTs encapsulating fullerenes in a simple vapor phase reaction by doping with C60 after an appropriate treatment of SWNTs (this symposium). The encapsulation of fullerenes succeeded equally well with various higher fullerenes and metal-endohedral fullerenes [Metal C60 Cm]95SWNT, where M is metal such as Gd, Lu, Sm, Sc, TEM and EELS revealed clearly individual metal atoms inside carbon cages [3]. These fullerenes aligned so regularly inside the central hollows of SWNTs that they can be considered one-dimensional fullerene crystal. Such SWNTs will behave differently in their physical and chemical properties from conventional ones, providing a new series of hybrid structures of fullerenes and nanotubes. Some of their properties will be presented. Other aspects of SWNTs encapsulating fullerenes are concerning structural evolution of encapsulating fullerene molecules themselves within the central hollows of SWNTs. We observed this encapsulated fullerene molecules can be fused together at an elevated temperature to form a smaller diameter SWNT inside the host SWNTs, leading to double-walled carbon nanotubes [DWNNTs] [4]. In our ex situ heating, the DWNNTs were formed in a high quantity so that their Raman signals showed clearly a characteristic correlation among Raman peaks. The formation of DWNNTs inside existing SWNTs does not involve any catalytic metal and thus their growth mechanism is simpler, providing useful information for the growth of SWNTs.

3) K. Hirabayashi, et al, Phil. Mag. and Reviews Letters, accepted.

11:15 AM A16.3 

STATISTICAL MECHANICS OF NANOEPAPODS. Miroslaw Hodkiewicz, Louis A. Girifalco, Dept of Material Science and Engineering, University of Pennsylvania, Philadelphia, PA.

A one dimensional lattice gas model is used to study nanoeapods. We study two different situations: Equilibrium of internal bucky balls with bucky balls outside in the gas phase and the equilibrium of bucky balls in close nanotube. By studying the open system we can determine conditions at which the nanobucky balls can be filled with bucky balls, whereas the closed system can give us information about clustering of internal bucky balls. By mapping the lattice gas model onto the one-dimensional Ising model, the partition function for the open system can be solved exactly, however using the same procedure, the closed system cannot be solved exactly, so we use the Monte Carlo method. Our results show that tubes can be filled very efficiently at room temperature provided we have enough external bucky balls in the gas phase. For a closed system at room temperature we found a high degree of clustering which decreases with increasing temperature. At about 500K the system goes from a quasi-solid into a quasi-liquid state. Because of the strong interaction between bucky balls, the system is far from its random state even at 1000K - the highest temperature studied. These results are in agreement with the experimental observations.

11:30 AM A16.4 

OPTICAL PROPERTIES OF ONE-DIMENSIONAL FULLERENE CHAINS ENCAPSULATED IN SINGLE-WALL CARBON NANOTUBES. M. Kodama, Y. Mizuno, Tokyo Metropolitan Univ., Dept of Physics, Tokyo, JAPAN, K. Hirabayashi, K. Suzuki, S. Iijima, Japan Science and Technology Corp, ICP, Nagoya, JAPAN, T. Kodama, K. Kikuchi, S. Suzuki and Y. Adachi, Tokyo Metropolitan Univ., Dept of Chemistry, Tokyo, JAPAN.

Single-wall carbon nanotube encapsulating fullerenes (peapod) is an interesting material as a new solid phase of carbon constructing a hierarchical spatial structure. We present zero to one-dimensional properties of [11,10] nanotubes as a simple example. A theoretical calculation shows some flat electronic bands for [11,10] nanotube encapsulating C60 chains. However, no one succeeded to measure optical properties of peapods to date. We realized high-yield fullerenes encapsulated in single-walled nanotubes using diameter selected nanotubes and specified fullerenes. HiTEM and electron diffraction reveals very high density packing of fullerenes inside single-walled nanotubes. At room temperature, time-resolved Raman spectra of C60 in peapods indicate photo- polymerization inside nanotubes by laser irradiation. Photo-polymerized C60-peapod show a similar Raman spectrum to that of the orthorhombic polymer phase. [5] At 4.2 K, however, no photo-polymerization reaction was observed. Single-rotations of C60 molecules play an important role for the photo-polymerization, this result suggests that even in one-dimensional space, C60 molecules have a similar spinning nature to those in thin films. In the case of C60-peapod, no photo-polymerization was observed. Observed Raman intensity of the C60-peapod is 1/10 of C60 films.

References:

11:45 AM A16.5 

DOPING AND/OR FILLING CARBON NANOTUBES WITH NITROGEN: AN EELS STUDY. Naoki Sugawara, Shinji Muto, Christian Collieux, Laboratoire de Physique de Solides, UMR 8522, Université Paris Sud, Orsay, FRANCE; Gilles Hug, LEM, ONERA-CNRS, UMR 104, Châtillon, FRANCE.

Synthesis of nanotubes containing nitrogen is attractive both for electronic and mechanical issues. The present study intends to investigate how far N atoms can be introduced into carbon based nanostructures, elaborated with different methods. Spatially and time-resolved EELS, respectively at the subnanometer and millisecond level, is used as a local probe of the composition and of the electronic structure. Using a dedicated FEG-STEM instrument, the CN-nanotubes grown by catalytic pyrolysis of gaseous precursors have been characterised by Electron Energy Spectroscopy (EELS) and High Resolution Transmission Electron Microscopy (HRTEM). High-resolution EELS line-scan show a modulated composition across the tube section with an increase in carbon on the external surface of the nanotube. Considering the individual spectra in more detail, it is observed that the π* peak of the C-K edge decreases with increasing concentration of nitrogen. The similar behaviour has previously been detected as well on CNx thin films grown by magnetron sputtering by chemical vapour deposition. The π* band of the C-K edge exhibits a similar shape to graphite close to the edge of the tube but becomes less structured when the nitrogen composition increases. It suggests that the structure consists of a graphitic stacking on the outside surface and an amorphous type CNx phase in the core. Furthermore, sequences of spectra recorded as a function of primary electron dose, rebuild that the insertion of the N atoms in the tube core may, in certain cases, be unstable, as demonstrated by the clear appearance of a N-K line characteristic of N2 molecules. We think the collaboration of our colleagues at the University of Sussex, Brighton, UK and the TEM CFST510B network.

SESSION A17: THERMAL AND TRIBOLOGICAL PROPERTIES

Chair: Rodney S. Ruoff
Thursday Afternoon, November 30, 2000
Grand Ballroom (Sheraton)

1:30 PM A17.1 

THERMAL PROPERTIES OF CARBON NANOTUBES. James Hose, California Institute of Technology, Dept of Physics, Pasadena, CA.

The thermal properties of carbon nanotubes reflect both their outstanding mechanical properties and their small size. The measured heat capacity of bulk samples of SWNTs is in excellent agreement with model calculations for individual nanotubes, and provides direct evidence of the quantization of the circumferential phonon wavevector. Detailed modeling provides a measurement of the energy spacing between LD phonon "subbands", and shows that the mechanical coupling between nanotubes in a bundle is weaker than expected. The thermal conductivity of SWNTs is high, and bulk samples of aligned SWNTs is within an order of magnitude that of crystalline graphite.

2:00 PM A17.2 

MESOSCOPIC THERMAL TRANSPORT MEASUREMENTS ON CARBON NANOTUBES. Philip Kim, Paul I. McEuen, Department of Physics, University of California, Berkeley, CA; Li Shui, Arunava Majumdar, Department of Mechanical Engineering, University of California, Berkeley, CA.

The thermal conductivity of nanotubes has been measured using a suspended mesoscopic device. The device was fabricated on silicon nitride membrane which is suspended above the substrate. It is connected to a thermal bath through a low thermal conductance path that isolates the heating and sensing elements. Carbon nanotubes
bridge two suspended structures to allow measurements of the thermal conductivity and thermopower of the tube. The observed thermal conductivity is consistent with the thermal conductivity of the gas layer.

2:15 PM A17.3
MECHANICAL AND TRIBOLOGICAL PROPERTIES OF CARBON NANOTUBES INVESTIGATED WITH ATOMIC SIMULATION
Samuel B. Soulen, Jr., University of Kentucky, Department of Chemical and Materials Engineering, Lexington, KY.

Experimental studies and computational simulations have shown that carbon nanotubes have mechanical properties that are both unique and potentially important for their use in new composite materials that could find use in structural applications. Most of the studies to date have focused on individual single-walled (SWNTs) or multi-walled (MWNTs) nanotubes. In this work we investigated the mechanical properties of SWNTs and MWNTs that have been filled with various gases, such as methane, xenon, and hydrogen, or clusters, such as buckyballs. The effect of the filling on the deformation of the nanotubes is examined with atomistic simulations using a many-body, reactive empirical bond-order potential that is coupled to long-range van der Waals potentials. The same method will be used to examine the tribological properties of SWNT bundles that are subjected to compressive and shear stresses between two sliding diamond surfaces. The simulations predict that the nanotubes are quite flexible and can therefore be subjected to high shear forces prior to wear. However, the precise nature of these responses is shown to depend on the orientation and attachment of the SWNT bundle with respect to the sliding surfaces.

2:30 PM A17.4
APPLICATION OF CARBON NANOTUBES AND FULLERENES FOR THERMAL MANAGEMENT
Leonard Yewell, Enrique Barrera, Rice Univ, Dept of Mechanical Engineering and Materials Science, Houston, TX; Brian Meyer, NASA Johnson Space Center, Houston, TX.

New techniques for thermal management in ceramics at the nanoscale level are proposed using low percentage of fullerene rich carbon nanotubes to control the degree of isotropy in thermal conductivity. Samples of yttria-stabilized zirconia containing fullerenes and nanotubes are prepared by tape casting and are characterized using the laser flash method, dimples and reduced thermal conductivity. Microstructural changes in zirconia due to the presence of fullerenes or nanotubes are related to differences in thermal conductivity and will be characterized using Raman, SEM, TEM, and XRD. Heat transport reductions normal to the sample surface will be analyzed and compared to previous research in thin ceramic-fullerene films to identify unique contributions to thermal management from the particle shape, size, and distribution. Support: Office of Naval Research Contract N00014-98-0-0246 and NASA Graduate Cooperative Education Program.

SESSION A18: FIELD EMISSION PROPERTIES AND APPLICATIONS
Chair: Hiroshi Tokumoto
Thursday Afternoon, November 30, 2000
Grand Ballroom (Sherraton)

3:15 PM A18.1
CARBON NANOTUBE ELECTRON SOURCES: EMISSION BEHAVIOR, ELECTRONIC STATES, AND CAP STRUCTURE
Kenneth A. Dang, Paul von Allmen, and Rishi R. Chahalwalla, Motorola Inc., Tempe, AZ.

Developing functional electronic devices based on carbon nanotubes requires a thorough understanding of fundamental electron emission phenomena in carbon nanotubes. To this end, we present recent results from field emission investigations of electron emission from individual single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs). Our experiments utilize a field emission microscope to observe nanoscopic phenomena occurring on nanotube tips under field emission conditions. We find that surface electronic states due to adsorbates dominate the behavior of both SWNTs and MWNTs under typical conditions and lead to current instability and current saturation. However, the behavior of clean, adsorbate-free nanotube surfaces is quite different. The field emission current is extremely stable, and the spatially-resolved field emission microscope images are related to the electronic structure of the nanotube cap. The field emission images of clean SWNTs and MWNTs are found to differ significantly. Clean nanotube surfaces also possess surface states that affect the tunneling current, as indicated by current versus temperature dependencies and electron energy distributions. We measure the maximum current per nanotube before field evaporation and show that through observation of the field evaporation, the nanotubes can be altered repeatedly to produce a set of different electron structures. We will discuss the impact of these properties on the performance of nanotube-based field emission devices.

3:45 PM A18.2
SYNTHESIS AND FIELD EMISSION PROPERTIES OF CARBON NANOTUBES
Chao Bao, Otto Zhou, Dept. of Physics, University of North Carolina; Wei Zhu, G.P. Kochanski, Sung-Ho Jin, Bell Laboratories, Lucent Technologies, Murray Hill, NJ.

We present our recent results on fabrication and characterization of cold cathodes based on carbon nanotube field emitters. The first portion of the talk will focus on the fabrication of carbon nanotube field emitters, while the second half will be devoted to the emission properties of these films. Specifically, we have successfully synthesized films consisting of well-aligned carbon nanotubes by microwave plasma-enhanced CVD. The nanotubes were found to nucleate and grow from catalytic oxide islands on a standard silicon wafer, with their diameters and lengths dependent on the size of the oxide islands. Electron microscopy revealed that the nanotubes grew via a base-growth mechanism, and studies of the growth kinetics revealed a very rapid initial growth that decreased sharply after the catalyst became fully encapsulated within the nanotube. A nucleation and growth model explaining our experimental observations will be proposed. Additionally, we present data that suggests the nanotube alignment was achieved by the plasma environment. We will show that nanotube films can be uniformly grown on concave surfaces with the nanotube alignment always perpendicular to the local substrate surface. We will compare the field emission properties of these films against the electron light emission. We will contrast the field emission properties of nanotubes with diamond and other types of cold cathodes, and consider the future of using nanotubes in vacuum microelectronic devices.

4:15 PM A18.3
CARBON NANOTUBE AND ITS APPLICATION TO TRIOID-TYPE FIELD EMISSION DISPLAYS

Carbon nanotube field emission displays (CNT-FEDs) have a strong potential to be applied to emissive devices including flat panel displays, cathode-ray tubes, back lights for liquid crystal displays, outdoor displays, and traffic signals. The CNT-FEDs have been demonstrated by our group based on the well-aligned nanotubes forming paste squeezer [1]. The fabricated displays were fully scalable and showed a high brightness on the green phosphor. The current fluctuation was found to be about 7% over a 9-inch panel [2]. In order to generate high quality moving images with high gray scale, low power consumption, and high brightness, the triode-type geometry should be realized. Here we report fabrication processes and field emission characteristics of a triode-type CNT-FEDs. The CNT cathodes were prepared by the paste squeezer and electrophoresis technique. A flat mesh gate electrode was inserted between the cathode and the anode plates. Uniform emission with high brightness was obtained. The electron emission was modulated at 1kHz at a bias voltage of 10630V. In this presentation, the effect of geometric factors upon the emission properties of the triode-type panel will be discussed together with the effects of fabrication process. [1] W.B. Choi, D. Chang, J.H. Kang, H.Y. Kim, Y.W. Jin, I.T. Han, Y.H. Lee, J.E. Jung, N.S. Lee, G.S. Park, and J.M. Kim, Appl. Phys. Lett. 75, 348 (1999). [2] W.B. Choi, W.S. Lee, H.S. Hwang, Y.W. Noh, B.G. Lee, N.S. Lee, J.E. Jung, J.H. You, M.J. Kim, The first 5-inch-carbon-nanotube-based field-emission displays for large area and color applications, SID 2000 Digest, pg221-222.

4:45 PM A18.4
ELECTRON EMISSION FROM PENTAGONS ON A CARBON NANOTUBE TIP REVEALED BY FIELD EMISSION MICROSCOPY
Koichi Hata, Akihiko Takakura, Yuki Saito, Meisei Univ, Dept of Electronic Engineering, Tsu, JAPAN.

Field emission of electrons from multiwall carbon nanotubes (MWCNTs) has been investigated in ultrahigh vacuum by field emission microscopy (FEM). MWCNTs whose tips are capped by curved graphite layers give FEM patterns consisting of bright pentagons, each of which has a dark region in the center. Several interference fringes are also observed between adjacent pentagonal rings. The
present result shows a direct evidence of the presence of 6 pentagons on a tip of a closed carbon nanotube. In previous FEM experiments performed under a poor vacuum, bright solid spots that were randomly distributed or arranged with two- and four-fold symmetry were observed. These bright spots are revealed to be due to adsorbed molecules such as oxygen on nanotubes tips. Adsorption of molecules seems to raise the tunneling probability of electrons.