Nanotubes - Science and Applications
Room 309 - Session NM+NS-MoM

Carbon Nanotubes: Functionalization and Applications
Moderator: P.M. Ajayan, Rensselaer Polytechnic Institute

8:20am **NM+NS-MoM1 Surface Interactions Used to Probe Metallic Carbon Nanotubes**, ***M. Dresselhaus,*** MIT **INVITED**

A brief overview will be given of the remarkable structure and properties of carbon nanotubes and how surface interactions are used for some of these studies. Carbon nanotubes are tiny structures of molecular dimensions in the form of hollow cylinders with about 20 carbon atoms around the circumference of the cylinders and microns in length. The unique electronic properties of carbon nanotubes are that they can be either semiconducting or metallic depending only on their geometry. From this, stem other remarkable and unique properties of their vibrational spectra, allowing us a means to distinguish metallic from semiconducting nanotubes in samples containing both. Interactions of the nanotubes with nanostructured metallic substrates have provided a powerful tool to gain a fundamental understanding about why the Raman spectra of metallic nanotubes are different from those for semiconducting nanotubes. Though less than a decade since their discovery, carbon nanotubes are already finding practical applications based on their unique properties.

9:00am **NM+NS-MoM3 Purification and Functionalization of Single-wall Carbon Nanotubes**, ***I. Chiang,*** *R. Saini, J. Margrave, R. Hauge, R.E. Smalley, R. Billups,* Rice University

A purification method has been developed which leads to 99.9% pure single wall nanotubes. It combines the well-known nitric acid treatment with water reflux and a two-stage gas-phase oxidation. Air oxidation of SWNTs is correlated to the amount of metals in the samples. For sidewall fluorinated SWNTs, two distinct types of C-F bonds have been observed, ionic and covalent bonds. These 'fluorotubes' have served as precursors for further substitution on the nanotubes, such as sidewall alkylation etc. The degree of substitution is found to correlate with the extent of covalent sidewall C-F bonding.

9:20am **NM+NS-MoM4 Chemical Functionalization of Single-Walled and Multi-Walled Carbon Nanotubes through Ion Bombardment: Predictions from Molecular Dynamics Simulations Nanotubes**, *B. Ni,* ***S.B. Sinott,*** The University of Kentucky

Molecular dynamics simulations have been performed to study the bombardment of single-walled and multi-walled (double and triple) nanotube bundles by CH@sub 3@@sup +@ ions at impacting energies 10, 45, and 80 eV. The reactive empirical bond order potential for hydrocarbons was used in the classical simulations.@footnote 1@ The simulations predict that there is a high probability of radical or fragment adsorption to the nanotube walls which could serve as precursors to the chemical functionalization of the nanotube walls.@footnote 2@ In addition, the simulations show that ion bombardment at 80 eV can lead to cross-linking among the single-walled nanotubes that could stabilize the bundle relative to shear. The multi-walled nanotubes are predicted to be stiffer to scattering than the single-walled nanotubes, leading to increased fragmentation of the incident ions at lower energies. The results are compared to preliminary experimental results for the ion bombardment of muli-walled nanotubes and found to be in good agreement. This work was supported by the NSF (CHE-9708049 and the NSF MRSEC at the University of Kentucky, DMR-9809686) and by the NASA Ames Research Center (NAG 2-1121). @FootnoteText@ @footnote 1@S.B. Sinnott, L. Qi, O.A. Shenderova, D.W. Brenner, in Chapter 1 of Volume IV of ADVANCES IN CLASSICAL TRAJECTORY METHODS, Molecular Dynamics of Clusters, Surfaces,Liquids, and Interfaces, Ed. W. Hase (JAI Press, Inc., Stamford, CT, 1999), pp. 1-26. @footnote 2@B. Ni and S.B. Sinnott, Physical Review B 61, 2000 (in press).

9:40am **NM+NS-MoM5 A Novel Mechanism of Hydrogen Storage in Carbon Nanotubes**, ***Y.H. Lee,*** *S.M. Lee,* Jeonbuk National University, Korea

We have carried out systematic calculations for hydrogen adsorption and storage mechanism in the nanotubes. Hydrogen atoms first adsorb on the tube wall in an arch type and zigzag type up to a coverage of @theta@=1.0, and are stored in the capillary as a form of H@sub 2@ molecule at higher coverages. Hydrogen atoms can be stored dominantly through the tube wall by breaking the C-C midbond, %with relatively low activation barrier of 1.51 eV, while preserving the wall stability of a nanotube after complete hydrogen insertion, rather than by the capillarity effect through the ends of nanotubes. In the hydrogen extraction processes, H@sub 2@ molecule in the capillary of nanotubes first dissociates and adsorbs onto the inner wall, and is further extracted to the outer wall by the flip-out mechanism. Our calculations describe suitably an electrochemical storage process of hydrogen, which is applicable for the secondary hydrogen-battery.

10:00am **NM+NS-MoM6 Local Solvation Shell Measurement in Water using a Carbon Nanotube Probe**, *S.P. Jarvis,* JRCAT-NAIR, Japan*; T. Uchihashi,* JRCAT-ATP, Japan*;* ***H. Tokumoto,*** JRCAT-NAIR, Japan

Oscillatory forces between two approaching surfaces in solvent have long been the subject of study due to their possible influence on any surface-surface interactions mediated through a liquid or in the presence of a fluid film. Of particular interest is water, due to its omnipresence in all but the most stringently controlled environments and its role as the primary medium for biological interactions. Combining a carbon nanotube probe with an AFM has enabled us to measure oscillatory forces in water on approaching a surface that has been laterally characterized on a nanometer scale. One important aspect of the utilization of carbon nanotubes as the AFM probe is to remove the unwanted hydrodynamic damping effect caused by the bulk of the tip. We used a multi-walled carbon nanotube attached to a PtIr coated silicon lever in a specially designed FE-SEM. Another aspect is the usage of a magnetically activated AFM, which has been possible to resolve molecular layers of large molecules. With this method, magnetic material is deposited directly behind an AFM tip on the back-side of the cantilever so that the tip position can be controlled by the addition of a magnetic field. The lever can be vibrated in an oscillating magnetic field in order to make dynamic measurements. This success opens up the possibility of investigating water layers under a variety of experimental conditions and as a function of precise lateral position on any surface including biological membranes and macromolecules. Among the many and varied roles of water layers are effects on biomolecular adhesion, colloid dispersion and tribology, which can now be investigated with nanometer lateral resolution.

10:20am **NM+NS-MoM7 Single Wall Nanotube Probes for Structural and Functional Imaging in Fluid**, ***L. Chen,*** *J. Hafner, C. Cheung, C.M. Lieber,* Harvard University

Scanning force microscopy is a powerful tool for probing nanometer scale objects in fluid, ambient and vacuum environments. The contrast of SFM is based on the interaction between surface and probe which is additive over a wide spectrum of forces including Van der Waals, electrostatic and magnetic forces. Therefore, the resolution of SFM imaging greatly depends on the geometrical and mechanical properties of the probes. Carbon nanotubes make potentially ideal tips for SFM. First, carbon nanotubes can give unprecedented high resolution in structural imaging because of the intrinsic small diameters, high aspect ratio and reversible buckling. Second, carbon nanotubes can be functionalized to give chemically well-defined SFM probes, which enables functional or chemically sensitive imaging. Here we report recent progress in addressing critical issues associated with nanotube probes including the preparation of nanotube tips, structural imaging in fluid, and the functionalization of nanotube ends. Nanotube probes have been prepared by chemical vapor deposition (CVD) on commercial cantilever-probe surfaces. CVD nanotube probes have been used to image individual molecules of supercoiled DNA plasmid pBR322 on mica-fluid interface with high resolution. The relaxation of the supercoiled molecules was observed in real time in aqueous buffer solution. The chemical functionality of the nanotube end group was identified as carboxylic groups, by carrying out force titration experiments. Nanotube probes have been functionalized with synthetic oligonucleotides, and the resulting probes were capable of recognizing complementary oligonucleotide strands on surfaces. The force needed to unbind the 14 base pair duplexes was shown to be 450pN, which is in agreement with previous chemical force microscopy measurements.

10:40am **NM+NS-MoM8 Nonlinear Optical Properties of Some Polymer/Multi-walled Carbon Nanotube Composites**, ***Z.X. Jin,*** National University of Singapore, Singapore*; X. Sun, G.Q. Xu, S.H. Goh, W. Ji,* National University of Singapore

Several polymer-coated and polymer-grafted multi-walled carbon nanotubes(MWNTs) were synthesized and characterized using TEM and HRTEM. The polymer-coated or polymer-grafted MWNTs formed stable solutions in DMF. Their nonlinear optical properties were investigated using 532 nm nanosecond laser pulses. These polymer-MWNT composites still possess strong nonlinear optical properties.

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