

Tuesday Afternoon, November 5, 2002

Nanotubes: Science and Applications Topical Conference Room: C-209 - Session NT-TuA

Nanotubes: Mechanical Properties, NEMS

Moderator: L. Dai, College of Polymer Science and Polymer Engineering

2:00pm **NT-TuA1 Mechanics and Electrostatics of Nanotubes, D.W. Brenner, D. Areshkin, J.D. Schall, O.A. Shenderova**, North Carolina State University

INVITED

This talk will focus on modeling studies that have the aim of optimizing nanotube functionality in a number of applications, including nanocomposites and nanoelectromechanical (NEM) devices. The primary computational tools are a many-body bond-order potential energy function and a self-consistent hybrid density functional/tight binding scheme. The former is used for modeling structural and mechanical properties, including elastic properties of functionalized nanotubes. The latter method, which allows applied fields to be incorporated into a tight-binding Hamiltonian, is used to evaluate nanotube electrostatics and nonequilibrium electron transport. Topics to be discussed include the contribution of electrostatic interactions and nanotube polarizability to mechanical load transfer in nanotube-polymer composites, and alignment, kink formation and non-equilibrium transport in NEM devices.

¹ Funded by the Office of Naval Research and by NASA.

2:40pm **NT-TuA3 Carbon Nanotube/ Polymer Composite: Mechanical and Electrical Properties, H.Z. Geng**, University of North Carolina at Chapel Hill, *B. Zheng*, Duke University, *H. Shimoda*, University of North Carolina at Chapel Hill, *J.L. Liu*, Duke University, *O. Zhou*, University of North Carolina at Chapel Hill

Carbon Nanotubes with elastic modulus ~ 1 Tpa, and fracture strain $\sim 5\sim 10\%$, is interesting as filler for mechanical enhancement. Due to the poor dispersion and poor interfacial bonding between nanotube and polymer matrix, expected enhancement in mechanical properties by adding nanotube to polymer has by and large not been demonstrated. In this talk we present our results by using fluorinated nanotubes (F-SWNT). Differential scanning calorimetry (DSC) results show that our composite is macroscopically uniform. Tensile stress-strain curve and dynamic mechanical analysis (DMA) results show a significant enhancement of mechanical properties by adding only a few percentage of FSWNTs. Carbon black particle and carbon fiber filled polymer composites attract a lot of interest due to their Positive Temperature Coefficient (PTC) effect at percolation and therefore their potential application as temperature or current sensors. With large aspect ratio Carbon Nanotubes may offer some advantages over carbon black and carbon fiber, because percolation threshold is believed to be inverse of aspect ratio. In this talk we present our recent results on the dependence of percolation threshold on average length of nanotubes in CNT/polymer composites. Temperature effects on conductivities of composites at their percolations will also be presented.

3:00pm **NT-TuA4 Self-Aligned Mechanical Attachment of Carbon Nanotubes to Surfaces, K. Bylund, J.D. Whittaker, D. Kitchen, M. Housley, R.C. Davis**, Brigham Young University

We have investigated self-aligned transition metal silicides and other thin film deposition based processes for the mechanical attachment of carbon nanotubes to silicon surfaces. These processes could aid in the mass production of carbon nanotube based AFM probes and NEMS devices. In each process, thin films are deposited and processed to secure nanotubes to silicon surfaces. An investigation of the efficacy of these processes has motivated fundamental research on the interaction of carbon nanotubes with transition metals and their silicides at varying temperatures. We will present the effects of the metal deposition, silicide formation, and wet chemical etching on the films and the nanotubes as observed by scanning electron microscopy (SEM) and x-ray photoelectron spectroscopy (XPS).

3:20pm **NT-TuA5 Self-assembly of Carbon Nanotubes, S.J. Oh, H. Shimoda, H.Z. Geng, R.J. Walker, L.E. McNeil, O. Zhou**, University of North Carolina, Chapel Hill

Self-assembly is an efficient process employed by nature to fabricate higher-level architectures of micro- and nano- objects with controlled functionality. Here we report that pre-formed individual CNTs can self assemble into macroscopically ordered films and membranes. Electron microscopy and polarized Raman spectroscopy measurements indicate orientational ordering of the CNTs in these self-assembled structures, which

exhibit optical and electrical anisotropy. By controlling the functionality of the substrates, patterned CNT structures were obtained. Self-assembly of the CNTs is explained in terms of heterogeneous nucleation from a locally super-saturated suspension.

3:40pm **NT-TuA6 Fullerene Coalescence as a Junction Engineering for Nanoelectronics, B.I. Yakobson**, Rice University

Relaxation and failure¹ of C or BN² nanotubes can be reversed in a well-defined sequence of atomic rearrangements. This process corresponds to cap-to-cap coalescence or welding of two nanotubes. Precise mechanism is revealed by topological analysis³ and consists exclusively of number of Stone-Wales bond rotations, following the primary jump-to-contact polymerization with covalent bonding. This mechanism explains several "natural" phenomena like diameter doubling of nanotubes, coalescence of C₆₀ in peapods, etc. It also generates a series of stable intermediate neck-shaped hetero-junctions with potentially useful electronic properties due to electrostatic dipoles,⁴ density of states and conductance all varying along the series of emerging structures.

¹ B. I. Yakobson, Ph. Avouris, Topics Appl. Phys. 80, 287-329 (2001); Ge. G. Samsonidze, Gu. G. Samsonidze, B. I. Yakobson, Phys. Rev. Lett. 88, 065501 (2002).

² H. F. Bettinger, T. Dumitrica, G.E. Scuseria, B. I. Yakobson, Phys. Rev. B, 65, Rap. Comm., 041406 (2002).

³ Y. Zhao, B. I. Yakobson, R. E. Smalley, Phys. Rev. Lett., 88, 185501 (2002).

⁴ T. Dumitrica, C. Landis, B. I. Yakobson, Chem. Phys. Lett. (submitted).

4:00pm **NT-TuA7 Synthesis and Properties of Plasma-polymerized Polypyrrole / Au Nanotube Composite Structures, J. Zhou, E.R. Fisher**, Colorado State University

Composite nanostructures have a wide variety of potential applications in microelectronics, chemical sensors, and electrochemical energy production. Here, we report the synthesis of composite plasma-polymerized polypyrrole (PPPy)/Au nanotubes. The characteristics of both the PPPy films and the nanostructured composites have been investigated using FTIR, X-ray photoelectron spectroscopy (XPS), cyclic voltammetry (CV), and SEM. The gas phase species in the plasma have been investigated with mass spectrometry. The properties of PPPy films mostly depend on the applied plasma parameters, with both ring-opening reactions and the polymerization of pyrrole taking place simultaneously in the plasma. Decreasing the applied plasma power favors the retention of the rings of the pyrrole monomer. Mass spectra suggest that the plasma polymerization of pyrrole takes place on the substrate surface due to the diffusion of radicals produced in the plasma. In addition, thermal treatment after polymerization has been shown to enhance the conductivity of PPPy films. Thermally treated PPPy films can be partially oxidized or reduced electrochemically due to the exchange between cations and anions of PPPy films. From SEM analysis, it is apparent that reconstruction of PPPy films occurs after thermal treatment. However, non-thermally treated PPPy films coated on Au nanotubes demonstrate well-defined redox reversible peaks as results of the increasing of the interface areas between the surface of the PPPy films and electrolyte solution. The implications of these results for potential devices will also be presented.

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