# Friday Morning, October 29, 1999

## Topical Conference on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics
## Room 6C - Session NT+NS+EM+MS-FrM

### Nanotubes: Growth, Characterization and Properties II

**Moderator:** R.L. Jaffe, NASA Ames Research Center

8:20am **NT+NS+EM+MS-FrM1 Gas-phase Nanotube Production at High Pressure By Disproportionation of Carbon Monoxide**, ***P. Nikolaev***, G. B. Tech Inc. / NASA - JSC; *M. Bronikowski, K. Bradley, D. Colbert, K. Smith, R.E. Smalley,* Rice University

Single-wall carbon nanotubes (SWNTs) were produced in gas phase, in a flow tube reactor in 3 - 15 atm. of CO at 850@super o@ - 1200@super o@C. Nanotube growth was catalyzed by unsupported iron particles created in-situ by decomposition of iron pentacarbonyl vapor which was added to the CO feedstock at a few ppm level. We find that low Fe(CO)@sub 5@ concentration combined with fast heating rate of feedstock gas allows us to produce very small iron particles, while high pressure increases the rate of CO disproportionation, leading to effective nucleation and growth of SWNTs. Unlike pyrolysis of hydrocarbons, CO disproportionation is a "clean" process which proceeds only on the catalyst surface, resulting in essentially no amorphous carbon overcoating. Diameter distribution of the SWNTs is rather narrow and depends on CO pressure. Higher CO pressures (10 atm.) yield smaller nanotubes, with distribution centered at 0.7 nm (which is roughly the size of C@sub 60@ molecule). Nanotube yield relative to the amount of iron catalyst increases as the heating rate and mixing of Fe(CO)@sub 5@ are enhanced, indicating better catalyst utilization. In order to further increase nanotube yield, we have designed a "shower head" injector, in which cold CO/Fe(CO)@sub 5@ feedstock enters furnace through water-cooled injector, surrounded by "shower head" carrying CO pre-heated to 1200@super o@. Nanotube yield is also increased by addition of small amount of methane, while more CH@sub 4@ results in amorphous overcoating on the nanotube surface. In contrast to previously reported SWNT production methods, this scheme constitutes a continuous flow gas phase SWNT production process. It should therefore be readily amenable to scale up for bulk SWNT production.

8:40am **NT+NS+EM+MS-FrM2 The Optical Properties of Carbon Nanotubes and Their Use in the Characterisation of Bulk SWNT Material**, ***M.S. Golden***, *T. Pichler, R. Friedlein, M. Knupfer, J. Fink,* IFW Dresden, Germany; *O. Jost, A.A. Gorbunov, W. Pompe,* TU Dresden, Germany

The investigation of the optical properties of carbon nanotubes,@footnote 1,2@ either using UV-Vis or electron energy loss spectroscopies, offers insight into carbon nanotubes on two levels. Firstly, analysis of the energy positions of the characteristic electronic transitions between the singularities in the density of states enables a quick and easy determination of the overall NT yield, the diameter distribution and the ratio of semiconducting-to-metallic SWNTs in bulk samples. This represents an ideal express characterisation method to accompany tuning of the nanotube preparation process parameters. Secondly, the momentum dependence of the collective excitations of the @pi@-electron system in nanotubes measured using high resolution electron energy loss spectroscopy in transmission proves to be a sensitive probe of the effective dimensionality of the electron system and inter-tube interaction, both in bulk samples of SWNT and MWNT. @FootnoteText@ @footnote 1@ T. Pichler, M. Knupfer, M. S. Golden, J. Fink, A. Rinzler, R. E. Smalley, PRL 80 4729 (1998) @footnote 2@ T. Pichler, M. Sing, M. Knupfer, M. S. Golden, J. Fink, Solid State Commun., 109, 721 (1999).

9:00am **NT+NS+EM+MS-FrM3 Li Intercalated Carbon Nanotubes Ropes**, *J. Lu, J. Zhao,* ***A. Buldum***, *B. Gao, O. Zhou,* University of North Carolina, Chapel Hill **INVITED**

The electronic and electrochemical properties of Li intercalated single-wall nanotube ropes are studied theoretically using ab initio method@footnote 1@ and experimentally in an electrochemical cell.@footnote 2@ Complete charge transfer is found between Li atoms and nanotubes. The energetic and electrochemical potential of intercalated Li atoms on both the inside and the outside of tubes are investigated. The intercalated ropes are metallic with conduction band resides on C atoms. Both theoretical and experimental studies suggest that it is possible to achieve a Li intercalation density significant larger than that in the graphite, making the Li intercalated nanoropes a promising material for battery applications. @FootnoteText@ @footnote 1@ J. Zhao, A. Buldum, J. P. Lu, to be published. @footnote 2@ B. Gao and O. Zhou, to be published.

9:40am **NT+NS+EM+MS-FrM5 Mechanical and Electronic Properties of Carbon Nanotubes Under Bending**, ***L. Yang***, *M.P. Anantram, J. Han, R.L. Jaffe,* NASA

Bending, buckling and even collapsing of carbon nanotubes have been more frequently observed experimentally. They could be elastic or plastic deformations, and responsible for a variety of mechanical and electronic measurements. We systematically investigate mechanical and elecronical properties of carbon nanotubes under these deformations. They are correlated with tube configuration and stress - strain relations. Some interesting observations are made. For example, electron transport can be enhanced or suppressed, depending on the configuration and deformation of a tube. We also apply the simulation results in understanding some related experimental observations.

10:00am **NT+NS+EM+MS-FrM6 Effect of Strain on Electrical Properties of Carbon Nanotubes**, ***S. Paulson***, *N. Snider, M.R. Falvo, A. Seeger, A. Helser, R.M. Taylor III, R. Superfine, S. Washburn,* University of North Carolina, Chapel Hill

We have used an advanced interface to an Atomic Force Microscope to apply strain to carbon nanotubes. Simultaneously, we measure the current voltage characteristics, and see how they change as a function of strain in the tube. We have applied enough strain to fracture nanotubes, causing the resistance to become infinitely large, and then reassembled the ends to form junctions. The characteristics of these junctions will be discussed, as well as other strain dependant effects.

10:20am **NT+NS+EM+MS-FrM7 Molecular Dynamics Simulation of the Thermal Conductivity of Carbon Nanotubes**, ***M.A. Osman***, NASA Ames Research Center, US; *D. Srivastava,* NASA Ames Research Center

Carbon nanotubes (CNT) have very attractive electronic, mechanical, and thermal properties. Recently, measurements of thermal conductivity in single wall CNTs showed thermal conductivity magnitudes ranging from 17.5 to 58 W/cm-K at room temperature, which are better than bulk graphite.@footnote 1@ The cylinderical symmetry of CNT leads to large thermal conductivity along the tube axis which is an improvement over the strongly anisotropic nature of thermal conductivity of graphite. Additionally, unlike graphite, CNTs can be made into ropes that can be used as heat pipes. We have investigated the thermal concutivity of single wall CNTs Using non-equilibrium molecular dynamics (MD) with Brennar potential. The results of the simulation are in good agreement with the experimental results. We will discuss the results of our simluation and report on the effects of tube diameter and chirality on the thermal conductivity. @FootnoteText@ @footnote 1@ J. Hone, M. Whitney, C. Piskoti, and A. Zettl, Phys. Rev. B59, R2514 (1999).

10:40am **NT+NS+EM+MS-FrM8 Materials Applications of Carbon Nanotubes: Hydrogen Storage and Polymer Composites**, ***S.J.V. Frankland***, *D.W. Brenner,* North Carolina State University

Simulations addressing two applications of carbon nanotubes will be presented. Nanotubes have been proposed as storage media for hydrogen in fuel cells. Experiments have shown that the nanotube samples contain more hydrogen than will fit densely packed into the tubules themselves. Therefore, the location of the hydrogen is in question. The Raman shift of the hydrogen may provide a useful indicator of its placement. So far, two qualitative trends have been identified with molecular dynamics simulation which should enable the distinction of internal versus intercalated hydrogen. For internal hydrogen a decreasing Raman shift is observed with increasing nanotube radius. For intercalated hydrogen, the simulations predict a broadened Raman band with relatively little dependence on nanotube radius. The second application being considered is the usage of nanotubes to strengthen polymer composites. Molecular dynamics simulations are in progress to understand the load transfer mechanism between the polymer and the nanotube.

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