



NT09

**Tenth International Conference on the
Science and Application of Nanotubes**

<http://nanotube.msu.edu/nt09/>

**Tsinghua University
Beijing, China**

June 21-26, 2009

Keynote and Invited Presentations at NT09:

• Keynote lectures:

Phaedon Avouris	<i>(IBM Yorktown Heights, USA)</i>
Ado Jorio	<i>(Universidade Federal de Minas Gerais, Brazil)</i>
Hiromichi Kataura	<i>(AIST Tsukuba, Japan)</i>
Steven G. Louie	<i>(University of California at Berkeley, USA)</i>
Maurizio Prato	<i>(University of Trieste, Italy)</i>

• Invited talks:

Takuzo Aida	<i>(University of Tokyo, Japan)</i>
Arianna Filoramo	<i>(CEA Saclay, France)</i>
Achim Hartschuh	<i>(LMU Munich, Germany)</i>
Mark Hersam	<i>(Northwestern University, USA)</i>
Kaili Jiang	<i>(Tsinghua University, China)</i>
Jing Kong	<i>(MIT, USA)</i>
Kostas Kostarelos	<i>(University of London, U.K.)</i>
Zhongfan Liu	<i>(Peking University, China)</i>
Thomas Pichler	<i>(University of Vienna, Austria)</i>
Stephan Roche	<i>(CEA Grenoble, France)</i>
Kazu Suenaga	<i>(AIST Tsukuba, Japan)</i>

NT09 Program Schedule:

Time	Sunday 21 June	Monday 22 June	Tuesday 23 June	Wednesday 24 June	Thursday 25 June	Friday 26 June	
08:30		Registration					
09:00		Keynote 1: Ado Jorio	Keynote 2: Hironichi Kataura	Keynote 3: Steven G. Louie	Keynote 4: Phaedon Avouris	Keynote 5: Maurizio Prato	
09:45		Invited 1	Invited 3	Invited 6	Invited 8	Invited 10	
10:15	Registration Opens TUTORIALS	Intro Posters A	Intro Posters C	Contributed 18	Intro Posters D	Intro Posters F	
10:35		Posters A	Posters C	Break	Posters D	Posters F	
11:00				Invited 7			
11:30		Lunch	Lunch	Contributed 19	Lunch	Lunch	
12:30				Contributed 20			
12:50				Contributed 21			
14:00		Invited 2	Invited 4	Lunch	Invited 9	Invited 11	
14:30		Contributed 1 Contributed 2 Contributed 3	Contributed 8 Contributed 9	Excursion	Contributed 23 Contributed 24 Contributed 25	Contributed 30 Contributed 31 Contributed 32	
15:30		Intro Posters B	Contributed 10 Contributed 11 Contributed 12		Intro Posters E	Invited 12	
15:50		Posters B	Break		Posters E	Conference Summary	
16:00	Invited 5		Poster Awards				
16:10	Contributed 13						
16:30	Contributed 4 Contributed 5 Contributed 6 Contributed 7	Contributed 14 Contributed 15 Contributed 16 Contributed 17			Contributed 26 Contributed 27 Contributed 28 Contributed 29	Conference Conclusion	
17:45							
18:00							
19:00	Opening Ceremony and Welcome Party				Conference Dinner		

Color Legend:

Keynote lecture	Invited talk	Contributed talk	Contributed poster
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γ -Fe₂O₃ nanowire-filled carbon nanotubes with high efficiency filling ratio by plasma-enhanced chemical vapor deposition

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In recent years, carbon nanotubes (CNTs) filled with magnetic pure metal, alloy, metal oxide and metal carbide have attracted much attention for various technological applications ranging from magnetic data-storage devices, heterogeneous catalysis to ferromagnetic nanocontainers in biomedicines [1-3]. To date, two main methods are used for the synthesis of CNTs filled with metal oxide, namely the two-step method of wet chemical technique and one-step method of thermal chemical vapor deposition decomposition based on the pyrolysis of ferrocene [4-6]. In our present work, we introduce a simple method for in-situ synthesis of γ -Fe₂O₃ nanowire during CNT growth by plasma-enhanced chemical vapor deposition (PECVD).

Fe-Ni thin film with a thickness of 20 nm deposited on SiO₂/Si substrate by sputtering a Fe₅₀Ni₅₀ target was selected as the catalyst. For pretreatment of catalyst, the Fe-Ni alloy film was heated to 700°C for 40 min in a mixture of hydrogen, nitrogen and oxygen atmosphere in the PECVD chamber at pressure of 20 Pa. During in-situ growth of filled CNTs, feedstock methane was added in the mixture gas atmosphere at a flow rate of 80 sccm for 30 min, and the substrate temperature was maintained at 800°C. Scanning electron microscopy exhibited that the filling ratio in the CNT was higher up to 80%. High-resolution transmission electron microscopy, energy-dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy analysis confirmed the filling to be γ -Fe₂O₃ nanostructure.

References

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Contribution A.02 - Monday, June 22

NH₃ adsorption and dissociation on a nanosized iron cluster

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In doped nanotubes either or both boron and nitrogen atoms replace carbon atoms within the structure and are covalently bound. The main target is to control the electrical properties of the nanotubes, with special attention to control the number of layers. The important industrial potential is demonstrated by developing transparent, conductive, flexible nanotube mats. Despite widespread interest, the chemistry on the surface of BNC catalyst transition-metal nanoparticles is largely unknown though it is believed that the precursor molecules chemisorb dissociatively on their surface and there are major uncertainties in the carbon precursor surface decomposition reaction kinetics and the role of certain species which are believed to etch amorphous the nitrogen/carbon deposits from catalyst particles and thus permit surface decomposition reactions to persist for continuous BNC tube's growth [1,2]. We employed spin-polarized periodic density functional theory (DFT) [3] to study the bonding and chemistry of NH₃ and their fragment on a Fe₅₅ icosahedral cluster. We investigate the site preference for NH₃ with J. P. Perdew, K. Burke, and M. Ernzerhof (PBE) functional [3] and our results, which agree with recent experimental studies, suggest that for NH₃, only the interaction perpendicular at the cluster is favorable ($-0.37 \text{ eV} < \text{B.E.}(\text{NH}_3) < +0.05 \text{ eV}$). When the geometry optimization is started with the molecule placed flat on the surface, it's flipping up during the process. Anyway, also the perpendicular adsorption are not favourable when the hydrogen is toward the surface. Stable geometries of N and H on the high symmetry adsorption site of Fe₅₅ have been calculated as well. Both of the atom present similar behaviour: the hollow or top are the only stable sites and from the bridge sites, the adsorbed migrates on the nearest hollow site.

For the atomic nitrogen adsorption, FeN and Fe₃N conformation are observed. The most stable adsorption site is the hollow one (Fe₃N): -1.35 eV. The nitrogen on top sites bind to one iron and the interaction is less favourable: B.E.(N) = -0.05 eV.

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Contribution A.03 - Monday, June 22

Synthesis of shaped carbon nanostructures by high pressure CCVD: effect of nitrogen doping on their morphology and physical properties

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During last decade, various carbon nanostructures have attracted an increasing interest, due to their unique chemical, electronic, and mechanical properties, as well as many potential applications in drug delivery, chemical technology, magnetic data storage devices, and nanoscale electronics. The chemical inertness and capacious surface of these carbon nanostructures allows using them also as a new class of catalyst supports or nanoreactors. Selective formation of bulk amounts of various shaped carbon nanostructures such as nanoparticles (NPs), nanowires, single- and multi-walled carbon nanotubes (SWCNTs, MWCNTs) is one of the biggest challenges that needs to be solved for the future applications. Considerable efforts have been made in the recent years to develop methods for synthesis

of shaped carbon nanostructures with well-defined size and shape. Their properties depend on various factors such as size, crystal structure and surface doping. Nitrogen doping is a promising direction to improve properties of carbon nanostructures. It causes significant changes in their morphology, hardness, electrical conductivity, and chemical reactivity. Due to the incorporation of nitrogen in the graphene layers of carbon nanostructures, their properties are altered as compared to undoped ones.

For the synthesis of nanostructures, chemical catalytic vapor deposition (CCVD) method is a strong manufacturing route due to the ability of producing bulk amount of nanomaterial on a large-scale and controlling their structure more easily compared to other synthesis methods. In our work, we have developed a simple and effective method for preferential synthesis of nitrogen-doped SWCNTs, carbon-encapsulated metal NPs, or MWCNTs by the pyrolysis of gas mixture containing metallocene, acetonitrile and ethanol using high-pressure CCVD equipment. Conditions of formation such carbon nanostructures in dependence on the acetonitrile to ethanol ratio as well as other parameters (pressure, temperature) were determined. Morphology and chemical composition of synthesized materials were characterized by scanning and transmission electron microscopy, EDX, X-ray photoelectron and Raman spectroscopy. Electrical and magnetic properties of bulk amounts of synthesized nanostructures were analyzed using 2-point probe method and alternating gradient magnetometry, respectively.

Contribution A.04 - Monday, June 22

Secondary growth of carbon nanotubes by hot filament CVD without addition of catalyst

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Due to the ability to enlarge the surface area remarkably, the secondary growth of carbon nanotubes (CNTs) on primary CNTs has attracted growing interests for catalysis and sensor applications. It has also been found that the secondary CNTs can enhance field electron emission, and hold great potential in improving

uniformity and efficiency of field emission flat panel displays. A number of works have been done in growing secondary CNTs. However, addition of a catalyst is required in order to grow CNTs with different structure on the primary CNTs. To simplify the secondary growth process, it is in demanding to obtain secondary CNTs directly on primary CNTs without addition of any catalysts. In this work, the CNT growth was carried out using hot filament chemical vapor deposition in a gas mixture of methane and hydrogen. During the CVD processing, very low carbon concentration (0.28 vol. %) has been used to grow primary CNTs, and secondary CNTs growth on the primary ones has been achieved by simply increasing carbon source concentration to 5%. No catalyst was added throughout the whole processing. It was found that synthesizing primary CNTs at extremely low carbon concentration is the key for the secondary growth without additional catalyst. The mechanism for the secondary CNT growth and the field electron emission properties of resulted CNTs have also been investigated. Significant improvement of field emission properties has been observed due to the secondary growth of CNTs.

Contribution A.05 - Monday, June 22

Direct Growth of Aligned Carbon Nanotubes on Inconel Sheets and Their Field Electron Emission Properties

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Growth of carbon nanotubes (CNTs) directly from the substrates is of great importance in that it can pass over complicated and sometimes harmful post-processing for many CNT applications. Ni, Fe, stainless steel, and Ni based super alloys (Inconel) are usually used as substrates for direct growth of CNTs. Oxidation-reduction is an effective method for direct growth of CNTs, in which, alloy substrates were first oxidized in air then reduced in hydrogen environment before the thermal CVD process. However, the effect of the pre-treatment temperature on the formation of oxides and thus the quality of the resulted CNTs was not investigated. In this paper, direct growth of CNTs on Inconel 600 sheets was investigated using plasma enhanced hot filament chemical vapor deposition in a

gas mixture of methane and hydrogen. The Inconel 600 sheets were oxidized at different temperatures (800 °C, 900 °C, 1000 °C, and 1100 °C) before CNT deposition. The structure and surface morphology of the pre-treated substrate sheets and the deposited CNTs were studied by scanning electron microscopy and X-ray diffraction. The field electron emission (FEE) properties of the CNTs were also tested. The SEM results show that well aligned CNTs have been grown on the pre-treated Inconel sheets without addition of any catalysts and the higher treatment temperature resulted in CNTs with better uniformity, indicating that the oxidation pre-treatment of the substrate is effective to enhance the CNT growth. FEE testing shows that CNTs (grown on 1100 °C pretreated substrates) with better uniformity exhibit better FEE characteristics.

Contribution A.06 - Monday, June 22

Comparative study on carbon nanotubes synthesis with non-ferromagnetic catalyst mix in alcohol CVD

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The study of the magnetic properties of carbon nanotubes and the molecular hybrids based on them requires non-ferromagnetic pristine materials. However, in current state of the art the significant number of CVD carbon nanotubes synthesis is based on the ferromagnetic catalysts such as Fe, Co, Ni. Therefore, it is highly important to provide the optimized procedure for carbon nanotubes synthesis based on non-ferromagnetic catalyst mix. Additionally, the lack of the toxicity of the catalyst, if investigated in nanomedicine, would be an advantage.

In this contribution we present the systematic spectroscopic and microscopic studies on the synthesis of carbon nanotubes using e.g. copper or platinum supported on magnesia. Two catalyst precursors (platinum acetyloacetate and copper acetate) have been tested. Our findings show that the process parameters (alcohol - chemical vapour deposition A-CVD) influence the final morphology of the product significantly. Doublewalled carbon nanotubes and multiwalled carbon nanotubes have been synthesized using platinum based catalyst mix and bamboo-like multiwalled carbon nanotubes have been obtained applying copper based catalyst mix. The structure and the purity of the materials were investigated by means of

high resolution electron microscopy (HR-TEM) and Raman spectroscopy, respectively. The yield of the samples were determined via thermogravimetric analysis (TGA).

Contribution A.07 - Monday, June 22

Synthesis of Carbon Nanotubes by Thermal Chemical Vapor Deposition Method Using Thin Film Nickel Catalyst

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Carbon nanotubes (CNTs) were grown by pyrolysis of C₂H₂ using thermal chemical vapor deposition (TCVD) method and using mixture of different gases. Thin films of Ni, catalyst, were coated on SiO₂ substrate by ion beam sputtering. Because of using Ni catalyst, the pre-treatment in NH₃ environment was required for the CNT growth, which implies both the formation and the separation of the graphitic layer. We used H₂ for the dilution gas and C₂H₂ as the Carbon source. The effects of different parameters, such as temperature and time of growth were also studied in order to obtain satisfactory condition for growth of CNTs. These parameters were optimized in order to maximize the quality of CNTs. Scanning Electron Microscopy (SEM) was used to confirm the formation of CNTs and graphitized structures were confirmed by Raman spectra.

Contribution A.08 - Monday, June 22

Direct growth of vertically aligned carbon nanotubes by ferrocene-ethanol mist CVD and their application on ionization sensors

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In our previous work, parametric study of atmospheric-pressure single-walled carbon nanotubes growth by ferroceneethanol mist CVD was reported [S. Chaisitsak, J. Nukeaw, A. Tuantranont, *Diamond and Related Materials*, 16 (2007) 1958-1966]. Using this floating catalyst CVD technique, an uniform web-like single-walled CNT film could be deposited on various types of substrate at a low substrate temperature. In the present contribution, we extended the experiment to the formation of vertically aligned CNTs. The SEM results showed that the CNTs on bare substrates (alumina and stainless) were randomly aligned, while CNTs on aluminum-coated substrates were vertically aligned, indicating that aluminum is a suitable supporting layer for vertical growth of CNTs. A gas ionization sensor based on vertically aligned CNTs were also fabricated using a simple and low-cost technique. The breakdown voltages were measured at room temperature in different gases, such as He, N₂, Ar, O₂ and air. Sensor testing showed that the obtained devices had low working voltage (< 400 V), compared to similar devices reported earlier. Phosphor luminescent was also tested at 700~800 V in air by using Gd₂O₃S:Eu phosphor.

Contribution A.09 - Monday, June 22

Field Emission study of the carbon nanotubes growth mechanism.

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The outstanding properties of carbon nanotubes (CNTs) provide high potential for numerous applications. However, these properties are tightly related to the intimate structure of the CNTs. Accurate control of this structure is mandatory but not yet achieved in the different synthesis methods. This lack of control most probably arises from an insufficient knowledge of the nucleation and growth mechanism at the atomic level. The goal of this study is to image and chemically probe model catalysts at the nanoscale in CNTs CVD conditions, aiming at unraveling the initial stages of the still unknown growth mechanism.

In the present work(1), field ion and electron emission microscopies (FIM and FEM) are used to image model catalysts (Ni or Fe 3D single nanocrystals conditioned as sharp tips) in CNTs CVD growth conditions (873K, C₂H₂ or C₂H₅OH), *in situ* and at the atomic scale. At 873K, when the carbon containing gas is introduced into the chamber, the catalyst is observed to switch from a strongly faceted shape, as obtained in presence of H₂, to a new morphology presenting a considerably higher concentration of step-sites. The driving force of this morphological change is thus provided by carbon adsorption into energetically favorable step edges. Once the surface carbide is formed, graphitic nucleation is observed to start precisely at these carbon-enriched step sites.

In another set-up, the chemical composition of the surface was locally probed while this phenomenon was occurring. This set-up consisted of an atom-probe, which is basically an FIM connected to a ToF mass spectrometer. The selected probed area covered the (113) step-containing crystal plane. NiC_x compounds are observed in the spectra confirming the formation of a surface carbide. Carbon species are collected as C₁, C₂ and C₃ ions. The formation kinetics of these species has been studied by varying the reaction time between the probing field pulses and led to the conclusion that C₂₋₃ formation, by recombination of C atoms, is overall rate-determining. We thus suggest to consider them as potential building-blocks in the growth mechanism of CNTs.

Our nano-scale experimental approach answers essential questions of the growth mechanism of CNTs: (i)catalyst particles have to find a suitable shape, associated with surface carbide formation and step-sites creation, before any graphitic carbon nucleation can occur, and (ii), surface recombination phenomena lead to carbon dimers and trimers which could then act as building blocks during growth.

(1) M. Moors *et al.* , ACS Nano (2009), *In Press* .

Contribution A.10 - Monday, June 22

Impact of Molecular Structures of Carbon Sources in the Gas Phase CVD Growth of SWCNTs

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Although chemical vapor deposition (CVD) growth of single wall carbon nanotubes (SWCNTs) is a promising process, its growth mechanism has not been fully understood yet. Detection of many hydrocarbons as byproducts in the exhaust gas¹⁻³ indicates that the analysis of gas phase and surface reactions is important to understand the growth process in detail.

As a starting point to investigate elementary reactions of the SWCNT growth, intentionally nine aromatic hydrocarbons have been selected as carbon sources. Those hydrocarbons mainly differ in functional groups especially in terms of C-C bonding i.e. hybridization, attached to benzene rings in their structural formulas. Particularly, hydrocarbons having sp³ moieties are toluene, p-xylene, ethylbenzene and n-propylbenzene. Species having sp² moieties are styrene, allylbenzene and 1,4-divinylbenzene. Similarly species having sp moieties are phenylacetylene and 3-phenyl-1-propyne. Another noticeable point is the selection of an extremely dilute reaction condition, ~10⁻⁴ molar ratio of feedstock to carrier gas H₂ to reduce the complexities in decomposition reactions. Production of SWCNTs in different quantities only from n-propylbenzene, styrene, allylbenzene and 1,4-divinylbenzene is remarkable. Similarity in the production of sp² C₂ radical/neutral species C₂H₃ /C₂H₄ was found in the careful analysis of thermal decomposition reactions of those species. On this basis, it seems reasonable to speculate C₂H₃ /C₂H₄ as the major precursor for SWCNT growth. To support this speculation, 5.0 sccm of C₂H₄ was supplied with each aromatic hydrocarbon as a secondary carbon source. Under this condition all hydrocarbons could produce SWCNTs except species with sp moieties. Resonance Raman and optical absorption spectroscopic analysis of as grown samples have also supported the importance of C₂H₃ /C₂H₄. These results clearly suggest that the molecular structure of the carbon source is a key factor in the CVD growth of SWCNTs.

References

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3. B. Shukla, T. Saito, M. Yumura, S. Iijima, Chem. Commun., in press.

Contribution A.11 - Monday, June 22

K-effect of carbon nanofibers synthesized from CO₂ on

Ni/Al₂O₃ by a catalytic hydrogenation reaction

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Chemical vapor deposition (CVD) has long been used to produce carbon nanofibers (CNFs) and carbon nanotubes (CNTs). Numerous transition metals such as Ni, Co, Fe, and their alloys have been shown to be efficient catalysts for CNF production. Carbon sources have included C1-C6 hydrocarbons such as CH₄, C₂H₄, C₂H₂, and aromatic compounds. Carbon dioxide, primarily generated from combustion, is the most important and abundant greenhouse gas, and it is the main contributor to the greenhouse effect. It has therefore become important to reduce the release of CO₂ and implement CO₂ recycling. To this end, chemical conversion of CO₂ by catalytic reaction has been recognized as one of the most promising processes for CO₂ utilization.

In this report, commercially available Ni/Al₂O₃ containing various concentrations of potassium has been used to achieve carbon deposition from CO₂ through catalytic hydrogenation. Experimental results show that K additives induce the formation of carbon nanofibers or carbon deposition on Ni/Al₂O₃ during the reverse water gas shift reaction. The carbon yield increases with increasing K content in the case of Ni/Al₂O₃ exposed to a feed of H₂/CO₂. We report here that the active sites on Ni-K/Al₂O₃ catalysts for carbon deposition from H₂/CO₂ depend on the presence of potassium K additives can interact with the nickel in Ni/Al₂O₃ to facilitate the formation of active sites that enable carbon deposition. The formation rate of carbon deposition is proposed to depend closely on an ensemble control, suggesting that the ensemble size necessary for carbon formation may also be ca. 0.5 potassium atom.

Contribution A.12 - Monday, June 22

Growing Multi-walled Carbon Nanotubes by Metal-Sulfate Catalysts

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We report a simple method to synthesize multi-walled carbon nanotubes (MWCNTs) on a reinforced filler-carbon black (CB) by metal-sulfate catalysts-FeSO₄, NiSO₄, CoSO₄ and CuSO₄ at different loading. MWCNTs are synthesized at 700~950 °C; by directly decomposing form diluted ethylene (C₂H₄/Ar) in the ratio of 0.05~1. The growth yield and rate of MWCNTs are depending on the surface properties of catalysts, reaction temperature and dwell times conducted in-situ by TGA measurements or in a high-temperature furnace. The surface morphologies of MWCNTs are examined by SEM, HR-TEM and RAMAN. The growth behaviors of MWCNTs over metal-sulfate catalysts are quite different from previous studies. Size control of metal particles are proposed not to be the decisive step for growing CNTs, the main factor would be controlled by surface morphology of metal catalysts.

Contribution A.13 - Monday, June 22

Multi-walled Carbon Nanotubes Synthesized by Different Methods

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Multi-walled carbon nanotubes (MWCNTs) were synthesized by thermal chemical vapor deposition (CVD), hot filament CVD (HFCVD) and microwave CVD (MWCVD) using Ni-Mg-Mo-O alloy oxides as catalyst. The resultant CNTs were characterized by transmission electron microscope (TEM) and Raman spectroscopy. The results reveal that the MWCNTs synthesized by different methods have different characteristics, probably attributing to different atomic hydrogen concentrations produced by different methods. High temperature plasma produces high concentration of atomic hydrogen to etch the amorphous carbon or defected CNTs formed during the processing, thus increasing the degree of graphitization and reducing the diameter of the resultant CNTs. In addition, MWCNTs were synthesized successfully at low temperatures (550 °C or below) using MWCVD due to

the enhancement of plasma in decomposition of methane and production of high concentration of atomic hydrogen at low temperatures.

Contribution A.14 - Monday, June 22

CCVD synthesis of C- encapsulated Co, Fe, Co/Fe and Ni nanoparticles for cancer treatment by hyperthermia. Magnetic properties and heating effect.

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In this work, we discuss the influence of different conditions of synthesis of C- encapsulated Fe, Co, Ni and Co/Fe. The magnetic properties and heating effect on these products are also compared. The investigated samples contain spherical and oblong carbon-encapsulated Co nanoparticles with size distribution 6-10 nm (60%) and 11-20nm (40%). Oblong or spherical carbon-encapsulated are observed for Fe nanoparticles with diameter within the range 1-10nm (80%) and 11-30 nm (20%). The encapsulated nanoparticles have been synthesized by catalytic chemical vapour deposition (CCVD) with gaseous mixtures of H₂/CH₄ or N₂/CH₄, using a MgO support coated with Mg_{0.95}Co_{0.05}O [1], Mg_{0.95}Fe_{0.05}O, Mg_{0.95}Ni_{0.05}O or Mg_{0.95}Fe_{0.025}Co_{0.025}O solid solutions. The analyses of the metal content in the final purified products (HCl washing for dissolution of the oxides) indicate 10 11 wt. % of Co, 7 13 wt.% of Fe, 4 wt.% of Ni and 8 wt.%

of Fe/Co. We observed that the gaseous mixtures of H₂/CH₄ give us higher Fe content and bigger C-thickness than N₂/CH₄ gas mixture. The magnetic characterization of encapsulated Co nanoparticles shows magnetization $M_S = 24$ emu/g, much higher than Fe, Ni or Fe/Co respectively $M_S = 16, 2$ and 11 emu/g. The heating effect of the Co product in suspension in water has been evidenced even at low power (30 kA/m) and low concentration (5mg/mL). The samples were characterized by TEM, Raman spectroscopy, elemental analyses, X-ray diffraction, VSM- SQUID magnetometer and AC- heating. This work is performed in the frame of the European FP6 RTN CARBIO (www.carbio.eu) which deals with bio-application of carbon nanotubes filled with magnetic materials for cancer treatment by hyperthermia.

Contribution B.01 - Monday, June 22

direct evidence for the lip-lip interactions in multi-wall carbon nanotubes

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The stability of open edged multi-walled carbon nanotubes has been investigated by using in situ high resolution transmission electron microscopy (HRTEM) at elevated temperatures. Formation of inter-shell structures was experimentally observed for the first time and attributed to a robust interaction between adjacent concentric shells (so-called lip lip interaction). The fluctuating behavior of the inter-shell structures suggests a mechanism by which the carbon atoms can pass in or out through the inter-shell edges during carbon nanotube growth or shrinkage processes.

Contribution B.02 - Monday, June 22

On the Role of the Metal Catalyst for SWCNT Nucleation and Growth Studied by Quantum Chemical Molecular

Dynamics Simulations

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Using the density-functional tight-binding (DFTB) electronic structure method, we have previously performed nonequilibrium quantum chemical molecular dynamics (QM/MD) studies on the mechanism of carbon nanotube (CNT) nucleation [1] and growth [2] on the (000-1) (C-face) of crystalline SiC during high-temperature vacuum decomposition. We found that the carbon released from the SiC crystal by silicon evaporation self-assembles into graphene sheets. On the C-face, the graphene interactions with the dangling bonds of the surface C atoms is strong enough to lead to the emergence of dome-shaped structures with circular shape (CNT caps) on the flat surface, since such cap structures maximize the surface area (and therefore minimize the graphene curvature). The CNT nucleation process in this case resembles somewhat the conventional VLS model where carbon precipitates from a crystalline or liquid metal carbide particle.

On the other hand, using DFTB-based QM/MD simulations, we have recently demonstrated that carbide formation is not necessary for continued growth of single-walled CNT (SWCNT) fragments when atomic carbon is supplied from vacuum, irrespective of whether straight tube sidewalls [3] or half-fullerene caps [4] were attached to an Fe₃₈ nanoparticle. Although these simulations employ transition metal catalysts, we note that, curiously enough, carbide formation is not immediately required to achieve sidewall growth if carbon is supplied from vacuum. A more important factor seems to be the mobility of the atoms on the Fe₃₈ surface. We will also discuss the effect of different carbon feeding rates on the hexagon purity of the constructed sidewalls.

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Contribution B.03 - Monday, June 22

Room temperature ionic liquid inside carbon nanotubes: the filling process and melting behavior

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What will happen when the low-melting ionic liquids are confined in the narrow hollow interior of carbon nanotubes? From the point of view of the unique properties of ionic liquids (including good electrical conductivity, high ionic mobility, wide electrochemical window, and high chemical and thermal stabilities), carbon nanotube filled with ionic liquid should be a new type of CNTs-based nanocomposite. It also offers a good opportunity to investigate the structure and phase variation of ionic liquid in nanometer-sized confinement.

In this study, we demonstrated for the first time the different morphologies of ionic liquids inside single-walled carbon nanotubes (SWNTs). A zinc contained quaternary ammonium based ionic liquid [Me₃NC₂H₄OH]⁺[ZnCl₃]⁻ (named as ChZnCl₃ for simplicity) was chosen to achieve better imaging contrast and resolution for high-resolution TEM observation. The arrangement of encapsulated ChZnCl₃ shows clear dependence on the diameter of SWNTs. With successively increasing the diameter of SWNTs ranging from 1.4 to 2.3 nm, the ChZnCl₃ patterns appear to be single molecular chains, double helix, zigzag tube and finally random tube. This phenomenon is an observable manifestation of the confinement effect on ionic liquids. Furthermore, the melting of the ionic liquid into nanofluid in SWNTs has been studied by in-situ TEM electron beam irradiation, this process can be compared with a high-temperature heat treatment. Considering the high conductivity and stability of the ionic liquids in SWNTs, the observed multiform morphology and unique melting process of the ionic liquid in CNTs can provide a good candidate for elucidating phase behaviors of liquids in confined system. It is also anticipated that our work will encourage theoretical and experimental studies that further the fundamental understanding of the physicochemical

properties of ionic liquids and the host-guest interaction within carbon nanotubes and other confined systems.

Contribution B.04 - Monday, June 22

Chemically Purified DNA-Carbon Nanotubes and Narrow Graphene Nanoribbons from Carbon Nanotubes

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Current synthesis methods for carbon nanotubes (CNTs) usually give a mixture of electronic types (metallic or semiconducting), which makes it impossible for the application of as made CNTs for electronics. The separation of semiconducting vs metallic CNTs and the transformation of CNTs to other materials with unique electronic properties have become important in the past few years.

First, I will discuss the purification of DNA wrapped single-walled carbon nanotubes (SWNTs) using chromatography method for the application of nano-electronics. Chromatography can separate SWNTs according to their diameter, chirality, and length and the separation efficiency decreased with increasing tube diameter when the ssDNA sequence $d(GT)_n$ ($n = 10\text{--}45$) was used. The separation efficiency was improved by using the new DNA sequence $(TTTA)_3T$, which can recognize SWNTs with the specific chirality (10,5). The chirality of the separated tubes was examined by optical absorption, Raman, photoluminescence excitation/emission, and electrical transport measurements. According to the electrical measurement, around 99% (10,5) tubes were enriched by using the new DNA sequence. The FETs composed of separated SWNTs in parallel gave an Ion/Ioff ratio up to 10^6 due to the single-chirality-enriched (10,5) tubes. This is the first time that SWNT FETs with single-chirality SWNTs have been achieved. The chromatography method has the potential to separate even larger diameter semiconducting SWNTs from other starting materials to further improve the performance of the SWNT FETs.

In the second part, I will present the unzipping of multi-walled carbon nanotubes (MWNTs) to form graphene nanoribbons (GNRs). The high carrier mobility

of graphene offers the possibility of building high-performance graphene-based electronics. The all-semiconducting nature of sub-10-nm GNRs could bypass the problem of the extreme chirality dependence of metal or semiconductor nature of CNTs in future electronics. Currently, making GNRs using lithographic, chemical or sonochemical methods is challenging. It is difficult to obtain GNRs with smooth edges and controllable widths at high yields. Because CNTs are considered to be GNRs rolled up into seamless tubes and the synthesis, size control, placement and alignment control of nanotubes have been widely investigated and established, we ask the question of whether CNTs can be unzipped to form GNRs with structural control. The greatest challenge in converting CNTs to GNRs is to develop ways of cleaving CNTs in the longitudinal direction without rapid etching along the circumference. Here we show an approach to making GNRs by unzipping MWCNT by plasma etching of nanotubes partly embedded in a polymer film. The GNRs have smooth edges and a narrow width distribution (1020 nm). Raman spectroscopy and electrical transport measurements reveal the high quality of the GNRs. Unzipping CNTs with well-defined structures in an array will allow the production of GNRs with controlled widths, edge structures, placement and alignment in a scalable fashion for device integration.

Contribution B.05 - Monday, June 22

CVD grown graphene on sapphire substrates

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Graphene is one of the most promising materials to open a new era of electrical and optical integrated circuit because of its unique electrical structure. Two new technologies are essentially required to apply graphene practically to electrical and optical devices. The first technology is a growth method of graphene on nm-order flat insulator layers to fabricate electrical and optical devices. The second one is band-gap opening method to obtain high on/off ratio of electrical devices and to realize optical devices.

We developed a new growth method of graphene on single-crystal sapphire substrates. The close-packed oxygen atoms on C-face sapphire are lattice-matched to graphene and it could be possible to grow graphene epitaxially on it. Our growth method is chemical vapor deposition (CVD) using acetylene as a source gas and nitrogen as a carrier gas. The growth temperature is 600-700°C in the atmospheric pressure.

We use a 2-inch sapphire substrate with polished surface on both sides to measure the optical transmittance of grown graphene layers. The growth thickness of the graphene layers is proportional to the growth time and the flow rate of acetylene assuming that the thickness of grown graphene layers is proportional to its optical absorbance. Despite their thickness, the optical transmission spectrum of CVD grown graphene layers shows that their transmittance increases gradually from the wavelength of 300 nm to 2700 nm. The domain size of our graphene is about 5 nm measured by a scanning tunneling microscope. The G/D ratio of Raman spectrum is 1.3 when the growth temperature is 700°C and 1.2 when the temperature is 600°C. Besides 2D and G+D bands, there is a small peak at 3200 cm⁻¹. It is reported that optical transmittance measurements of a freestanding monolayer graphene prepared by micromechanical cleavage of natural graphite flakes showed that the transmittance was 97.7% and it was wavelength-independent at least from 500 nm to 1200 nm [1]. The wavelength dependence of the transmittance of our graphene layers is attributed to their small domain size.

In conclusion, we developed a new growth method of graphene on sapphire substrates that is applicable to fabricate electrical and optical integrated circuit.

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Contribution B.06 - Monday, June 22

Individual Single-Wall Carbon Nanohorns Separated From Aggregates

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Single-wall carbon nanohorns (SWNHs) [1] are single-graphene tubules with diameters of 2-5 nm and 40-50 nm in length. About 2000 of SWNs assembled and formed a spherical aggregate with diameter of about 100 nm. Applications of SWNHs to drug delivery system [2-6], fuel cell, and gas adsorption have been studied and SWNHs are found to be potentially useful due to their unique structures.

We show in this report that individual SWNHs are separated from the as-grown SWNHs by applying sucrose density gradient centrifugation. Prior to this centrifugation, as-grown SWNHs were oxidized with air, dispersed in cholate solution, and sonicated. The obtained individual SWNHs were observed with transmission electron microscopy (TEM), and found that they were straight or branched (two- or three-ways). Analysis of TEM images showed that the numbers of straight and branched SWNHs were both about 30%. Most of the remaining 40% were small aggregates of SWNHs with sizes of 10 to 50 nm. Lengths of straight SWNHs or of arms of the branched types were 10-100 nm and their diameters were 2-10 nm. The inside spaces of the individual SWNHs were empty, where Gd₂O₃ nanoparticles were incorporated.

The individual SWNHs and small sized aggregates of SWNHs are unique in the shapes and sizes, and they are new classes of single graphene tubules. We believe that these new types of graphene tubules will be not only useful for as the drug carriers, but also open up new application possibilities of the graphene tubule objects.

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Contribution B.07 - Monday, June 22

Synthesis of Polygonal Carbon Nanocapsules by Arc Discharge Method

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The purpose of this study is to determine the physical and chemical properties of polygonal carbon nanocapsules (PCNCs) by arc discharge with thermogravimetry (TGA), powder X-ray diffraction (XRD), RAMAN spectroscopy (RAMAN), transmission electron microscopic (TEM) and temperature programmed oxidation (TPO) methods. PCNCs are easily to be found in the as-grown soot synthesized by arc-discharge with other carbon materials, such as carbon nanotubes, graphene and carbon black. Triangular, tetragonal and pentagonal forms of PCNCs are the main product self-assembled during the arc-discharge process measured by HR-TEM. The structural properties of PCNCs are hardly modified by acid-treatments over HNO₃ solution at 120oC or oxidized by oxygen at 750 oC evidenced by RAMAN, XRD, TGA , TPO and HR-TEM. The unique physico-chemical properties of PCNCs are similar to them of well-defined graphite or multi-layer graphene. The effective separation of PCNCs from as-grown soot is under studying.

Keyword: polygonal carbon nanocapsules, arc discharge

Contribution B.08 - Monday, June 22

Electrochemical Charging of Individual Single Walled Carbon Nanotubes

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Abstract

Control of the electronic structure of single wall carbon nanotubes (SWCNTs) is an important issue for their application in nanoelectronic devices. The electronic structure of SWCNTs can be changed by chemical doping, electrostatic or electrochemical charging (gating). However, the electrochemical charging is different from chemical doping. In the latter case, the redox active molecule (chemical dopant) can penetrate into the interior of the carbon nanostructures. In some cases (for example in fullerene peapods), the chemical doping is highly irreversible and the chemical dopant cannot be removed even by the extraction with a solvent. Electrochemical charging, on the other hand, mimics a double layer capacitor, where the charge carriers are injected into the nanotube from the electrode and the electrolyte ions only compensate the injected charge. In situ Raman spectroelectrochemistry is a well-established method for investigating the change in physical properties of SWCNTs during charging. In situ spectroelectrochemical measurements have been so far typically performed on large bundles of SWCNTs, which complicates the interpretation of spectra, since the individual properties of specific tubes are averaged. Furthermore, nanotubes in a bundle exhibit different properties as compared to those of individual nanotubes and the electrochemical charging is often inhomogeneous across the bundle. Therefore, it is desirable to focus attention on spectroelectrochemical studies of small bundles and ideally on individual carbon nanotubes.

Here we report the effects of electrochemical charging (gating) on the Raman spectra of SWCNTs as a function of their diameters and laser excitation energy. In contrast to SWCNT bundles, it is possible for individual tubes to find the dependence of the G+ mode frequency ω_{G+} on the diameter of the nanotube. During negative charging ω_{G+} can be either down shifted or up shifted. We show experimentally that this effect for semiconducting SWCNTs depends on nanotube diameter. The change of the sign of the frequency shift with applied potential ($\delta\omega_{G+}/\delta V_e$) is rationalized by a competition between two effects: namely, a phonon renormalization effect and a C-C bond weakening during the charging process. Furthermore, we show here the data on the development of the G+ mode during the positive charging of individual semiconducting SWCNTs. These electrochemical data cannot be obtained using a back gate due to the presence of trapped charges in the gate oxide.

STM simulations of B- and N-doped graphene and nanotubes

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The tuning of carbon nanotubes and graphene electronic properties are an important challenge for the design of nanoelectronic devices. The chemical doping is one of the possible methods to achieve such a controlled of electronic and optical properties. Beside the physical properties of modified carbon materials, the knowledge of the experimental fingerprints of doping configuration is crucial to analyzed the experimentally produced samples.

We have studied electronic properties and STM fingerprints of substitutional and pyridine-like doping by boron and nitrogen for graphene sheet and nanotubes in a Tersoff-Hamman formalism using density functional theory based calculations. These configurations are presently the most probable in doped carbon nanotubes. We observed that the STM fingerprints depend on the host graphitic network (planar or curved) and on the dopant configuration.

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Gate-controlled metal atom chains on graphene nanoribbons

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Electronic and magnetic properties of alkali and alkaline-earth metal doped graphene nanoribbons (GNRs) are studied with the use of pseudopotential density functional method. Strong site-dependence is observed in metal adsorption

on GNRs, and the adsorbed metal atoms are found to spontaneously form atomic chains on a particular form of GNRs. The magnetic properties of such doped GNRs exhibit intriguing features such as hysteresis and spin-compensation as metal atoms switch from one edge to another at alternating gate voltages. Our study shows that the metal atoms can be used as reagents that can identify the edge atomic structures of GNRs and also as gate-driven spin valves that control the spin current in GNRs

Contribution B.11 - Monday, June 22

Monitoring of healing process of electron beam irradiation induced defects on suspended individual single-walled carbon nanotube using micro Raman spectroscopy

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We have investigated the healing of defects on individual single wall carbon nanotube (SWNT) using micro Raman spectroscopy. The defects on the suspended individual SWNT were created by the low energy electron beam irradiation. The dose and the acceleration voltage dependence of the amount of damage were detected by the micro Raman spectroscopy. We found out that the repeated laser irradiation in the Raman spectroscopy could cure the electron beam irradiation induced damages on the SWNT. Suspended individual SWNT structure made it possible to make more sensitive and precise detection of defect production and healing process in the Raman spectroscopy. The amount of the damaging and the healing of the SWNT were measured by the observation of the peak intensity changes in both the radial breathing mode and the G-band mode.

Contribution B.12 - Monday, June 22

Characterization of DWCNT by Cs corrected TEM

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In the present study, Cs corrected TEM was used to characterize the CVD grown DWCNT. We will show the advantage and limitations of present method compared to existing methods.

Contribution B.13 - Monday, June 22

Doping effect of Al or P in carbon nanotubes

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Electronic, vibrational, chemical, and mechanical properties can be modified by doping carbon structures with either phosphorus (P) and/or Aluminum (Al).

In the case of pristine carbon nanotubes (CNTs), the electronic density of states is drastically modified, by adding or subtracting an electron due to doping effects [1]. Besides, it can also change the local chemical reactivity, as well as other properties. The capacity of change and control, it is of vital importance in nanostructures.

In this work we report a theoretical and experimental study on the effect of doping in CNTs with P or Al. Doped CNTs were produced in a gas reactor and characterized by different techniques. From theoretical side, density functional theory (DFT) calculations have been performed to study the effects of Al and/or P-doped armchair and zig-zag CNTs [2, 3]. For P-doped CNTs the density of states (DOS) is greatly modified, we had observed a change of metallic to semiconductor character in substitutional doping and low concentration. This result is

important because, we are interested in the possibility of changing the conduction properties in the CNTs, without a large modification of the mechanical properties. Finally we correlate the experimental with theoretical results.

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Contribution C.01 - Tuesday, June 23

The Effects of Structural Defects on the Dispersibility of Carbon Nanotubes in DNA Solutions

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Since DNA, a well-known biopolymer, has been proven to be effective for dispersing and sorting carbon nanotubes, intensive studies have been carried out in order to obtain both theoretical and experimental understanding of their interaction. In this study, we have studied the dispersability of carbon nanotubes in aqueous DNA solutions from the viewpoint of nanotube quality using optical spectroscopy. We found that the total amount of the dispersed as-grown defective tubes was two times higher than that of crystalline tubes thermally treated at 2300°C in argon. DNA was helically wrapped around the sidewall of the tubes in an irregular pattern. Based on the calculation of the density functional theory, defects on the sidewall of tubes provide additional sites for binding with DNA.

Efficient Separation of Single-Walled Carbon Nanotubes Having a Close Diameter

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Due to the difficulty in the synthesis of SWNTs with a specific chirality, SWNT chirality sorting has been an anticipated technique for realizing practical applications of SWNTs especially in the field of nanoelectronic devices since the properties of the SWNTs depend on their size and electronic structures. Density-gradient ultracentrifugation (DGU) is a powerful technique to separate SWNTs having a different diameter [1]. Separation of covalent-functionalized and non-functionalized SWNTs using the difference in their densities was reported [2], while fine sorting of SWNTs whose diameters are close is difficult.

Tetrachloroaurate was added to HiPco-SWNTs dissolved in a sodium cholate aqueous solution, and then DGU was carried out the solution was centrifuged with DGU. It was revealed that by this method, we can separate (6,5)-SWNTs from the other SWNTs including (8,3)-SWNTs. The present method is useful for the separation of the SWNTs whose diameters are very close.

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SEPARATION OF FUNCTIONALIZED SINGLE-WALLED CARBON NANOTUBES VIA FREE SOLUTION ELECTROPHORESIS SYSTEM

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This work presents the results of the separation of the functionalized single-walled carbon nanotubes (SWCNTs) by the free solution electrophoresis system. A raw single-walled carbon nanotubes were purified from an amorphous carbon and the residual catalysts by the initial annealing and three subsequent acid treatments in aqua regia solutions. Afterwards, the introduced functional groups and part of the defects were removed by high temperature annealing. Pristine carbon nanotubes were chopped in ultrasonication bath and splitted into two parts. One part of the material was dispersed in the water solution of sodium dodecyl sulfate (SDS) and the second part was dispersed in the water solution of polysorbate 20 (TWEEN 20). A well dispersed samples of wrapped carbon nanotubes were achieved by the sonication in ultrasound bath and subsequent stirring. Single-walled carbon nanotube samples were further functionalized with synthesised diazonium salt of the p-aminobenzoic acid. A selective introduction of the carboxylic groups onto carbon nanotube egzohedral surface via grafting process allowed the separation of the investigated material by its electronic properties. The metallic - semiconductive separation process of the functionalized single-walled carbon nanotubes was carried out in the free solution electrophoresis system (FSE). After the separation process a two fractions of the functionalized carbon nanotubes were collected and annealed in order to remove the introduced functional groups and restore the properties of the starting nanotubes. The efficiency of the separation of the functionalized single-walled carbon nanotubes by the free solution electrophoresis system was confirmed by the UV-vis-NIR spectroscopy. Additionally, the vibrational and chemical properties of the carbon nanotubes were investigated by the Raman spectroscopy and Fourier Transform Infrared spectroscopy (FT-IR).

Contribution C.04 - Tuesday, June 23

Synthesis and characterization of molybdenum nanowires encapsulating inside double-walled carbon nanotubes.

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Carbon nanotubes have known to be suitable template materials for preparation of new one-dimensional structure such as metallic nanowires, because the interior space of carbon nanotubes possess extremely small and long confined nano-space. In this study, we report synthesis of molybdenum nanowires encapsulating inside thin double-walled carbon nanotubes (less than 1nm) using simple solution method and characterization of the properties by HR-TEM, SEM, Raman, TGA, XPS, and nitrogen gas absorption.

Contribution C.05 - Tuesday, June 23

Open and Closed Edges of Graphene Layers

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Graphene, a single layer sheet of graphite, is the basic structural element of all other graphitic materials such as graphite, carbon nanotubes and fullerenes. The potential applications in condensed matter physics and electronics have boosted interest in graphene especially in the structure and properties of its edges. Recent studies indeed clarified the unconventional electronic features of graphene not only the monolayer but also the bilayer graphene sheet. Folding of monolayer and bilayer graphene, i.e. closed edges, were also studied by using the transmission electron microscope (TEM), however, no confirming evidence for the presence of open edges has been so far provided. Neither has the actual edge structure of graphene ever been atomically revealed. In this study, we report direct imaging of the edges of thermally treated graphite and show the evidence for a coexistence of closed and open edges in graphene. A high-resolution transmission electron microscope (HR-TEM) was operated at 120kV with a point resolution better than 0.106 nm. The method for determination of monolayer or more than one layer graphene sheets is established. Bilayer graphene with AA stacking has been carefully distinguished from a monolayer graphene by means of a series of tilting experiments. Open edge structures with carbon dangling bonds can be found only in a local area where the closed (folding) edge is partially broken.

Computational study of boron nitride nanotube synthesis: effect of catalyst morphology in stabilizing the boron-nitride bond.

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Together boron and nitride form similar structures as carbon. Graphene-like sheets and nanotubes have been demonstrated to exist with experiments and calculations [Golberg, et. al., *Advanced Materials* 19 2413 (2007)].

Boron Nitride NanoTubes (BNNTs) have very similar structure to Carbon NanoTubes (CNTs) and they possess impressive mechanical properties (for example, the Young's modulus is of the order of terapascals), while some of the BNNT properties are even more attractive than those of their carbon counterparts: CNTs are either conducting or semiconducting, while BNNTs are always semiconducting, allowing to produce semiconducting nanotubes only.

Boron nitride is also chemically very inert and resistant to oxidation, making it more attractive for applications such as shielding and coating. BNNTs, inheriting these same properties, might then serve as semiconductive coatings in harsh environments.

Despite of all these prospects, BNNTs have received, compared to CNTs, very little attention, mainly because their synthesis has proven to be quite difficult. This difficulty to synthesize BNNTs (and similar structures) when compared to their carbon counterparts is somehow intuitive. In CNT synthesis, according to microscopic models, individual carbon atoms diffuse on a catalytic nanoparticle, eventually forming cages and tubes. In the case of boron and nitrogen we have two different atomic species and this could lead to several undesirable end products instead of the desired boron-nitride bond.

Our aim is to study computationally the stabilization of the boron-nitride bond on a catalyst. In general, we are interested in how the nanoparticle topology (flat region versus highly coordinated catalyst atoms) and nanoparticle material affect

the formation of the boron-nitride bond when compared to other undesirable by-products (for example, N₂ and B₂). Our results for the iron catalyst show that the step edge stabilizes the boron-nitride bond, while in a close-packed catalyst regions, boron starts to form clusters with iron, spoiling the synthesis.

Contribution C.07 - Tuesday, June 23

Formation of nanocomposites using carbon nanotubes as fillers, and their application in NEMSs devices

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Organic thin film coatings are traditionally used as protective barriers for the more expensive systems underneath. However, progress in carbon based active nanoelectronic systems, in particular when combined with a filler material, has led to significant developments in many fields including display technologies, solar cells and new NEMS devices. The promise of using Fullerenes and polymers as the active media for electronics is far closer to realization once the mechanisms and process in forming the composite are fully understood using Raman and transport mechanisms. Additionally, in order to achieve very high conductivities (beyond 1000 s/cm) aspects of dimensionality and percolation need to be re-addressed. I shall discuss the progress in all these areas, but will focus on new NEMS built from polymer/nanotube coatings that can be used as EMI shields, strain transducers and non-metallic based antennas as well as our work on field emission from aligned nanotubes in a nanocomposite complex.

Contribution C.08 - Tuesday, June 23

Nanogears, cradles, hammer-like, and blade-cutting graphene-carbon nanotube composites

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Graphene-carbon nanotubes composites were considered as mono- and/or multiderivative structures when both tubes and graphene served either as main bodies or were attached additives. The composites were synthesized computationally in the framework of the unrestricted broken spin-symmetry approach implemented via the Hartree-Fock approximation. Computed profiles of the atomic chemical susceptibility (ACS) along the tube and across their body as well as over graphene sheets served as quantified pointers that allowed localising the most active contact zones of interacting partners.

Two SWNT fragments presenting (n,n) and (m,0) families, namely, (4,4,) and (8,0) and a set of NGr_s (n_a, n_z) (n_a and n_z match the number of benzenoid units on the armchair and zigzag edges of the sheets) were chosen to reveal general tendencies of the composite formation. Due to the fact that the space of chemical reactivity of both CNTs and graphene coincides with the coordinate space of their structures, addition reactions that lead to the composite formation are not local but largely extended in the space. This greatly complicates the construction of starting diads, triads, and more complex configurations of components making their number practically endless. However a thorough analysis of ACS profiles of both components made it possible selecting two main groups of the composites, conditionally called hammer and cutting-blade structures. The former follows from the fact that empty ends of SWCNTs are the most chemically active so that the tubes might be willingly attached to any NGr forming a hammer handle. The latter is a consequence of exclusive chemical reactivity of both zigzag and armchair edges of non-terminated NGr, so that NGr can touch a SWCNT sidewall as a blade. As occurred, the coupling energy of cutting-blade composites exceeds that of hammer ones that is important for a practical realization of the composites production. The final product will depend on whether both components of the composition are freely accessible or one of them is fixed. Thus, in diluted solutions (in polymers [1, 2]) where the first requirement is met, one can expect the formation of the multi-addend cutting-blade composites (peculiar gears) due to significant preference in the coupling energy. Among the latter, a particular cradle composite is suggested for an individual graphene sheet to be fixed by a pair of nanotubes. Oppositely, in gas reactors where often either CNTs or graphene sheets

are fixed on some substrates, the hammer composites will be formed as it has been shown just recently [3].

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Contribution C.09 - Tuesday, June 23

Investigation of the interaction between carbon nanotubes and metal nanoparticles

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Carbon nanotube field effect transistors (CNTFET) are known to interact with various airborne and fluidic materials and such interactions are being utilized to develop highly sensitive sensors. Understanding the mechanism of these interactions therefore becomes important towards the design and successful realization of such sensors. Gold nanoparticles decorating carbon nanotube FETs have been proposed to serve as a good linker in thiol-based bio-functionalization, and they are also reported to modify the transport property of the nanotube ^[1]. This work will investigate the mechanism of the transport modification, and specifically, whether it occurs through charge transfer or contact-to-nanotube barrier alteration.

The CNTFET devices in this investigation use isolated single-walled nanotubes, and the metal nanoparticles are deposited through an electrochemical process. Three types of devices are used: 1. CNTFET with both CNT and metal contact areas decorated with metal nanoparticles; 2. CNTFET with the nanotube protected by PMMA, with only the metal contact region decorated with metal nanoparticles; 3. CNTFET with metal contacts PMMA protected, and only the nanotube decorated with metal nanoparticles. For all types of devices, the transport property measurements are taken before and after the metal nanoparticle deposition. Through comparison of the changes in transport property of the different types of device,

the mechanism of the interaction between CNT and metal nanoparticle can be elucidated.

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Contribution D.01 - Tuesday, June 23

Application of Carbon Nanotubes in Nuclear, Particle and X-Ray Physics

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After the first consideration [1] of the possible use of carbon nanotubes in high energy and X-ray physics based on the unique properties of nanocrystals and bundles of carbon nanotubes, many theoretical and numerical works devoted to this problem have been published by Lyon-Moscow-Kharkov-Yerevan collaboration and other groups (see the review [2]). Experimental results on nanotube based detectors sensitive to UV [3] and IR [4] photons, as well as proposals [5] for the use of single nanotubes for beam particle monitoring and for construction of ionization counters for separate particles also are available. In this invited talk the physical principles of such applications are discussed, a review of the published works and construction of the corresponding devices and detectors are given.

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Contribution D.02 - Tuesday, June 23

Use of Single Carbon Nanotubes for Beam Particle Monitoring and Detection of Separate Charged Particles

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The nanocrystals and bundles of carbon nanotubes can be used for various applications of high energy and X-ray physics [1]. In this work it is shown that due to unique physical properties, namely, high Young's Modulus and good electrical and thermal parameters, the single nanotubes also can help to solve many actual problems of beam particle monitoring and detection of separate particles if some difficulties connected with manipulation with already produced long nanotubes will be overcome. The physical principles, construction and advantages of nanotube beam monitors as well as of single wire and multiwire ionization counters measuring the ionization, coordinates and other parameters of separate high and low energy particles are discussed.

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Contribution D.03 - Tuesday, June 23

Carbon Nanostructures as Deformation and Reaction Cells

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Carbon Nanostructures as Deformation and Reaction Cells

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Keywords: Carbon nanostructures; Electron irradiation; In-situ electron microscopy

Concentric closed-shell nanostructures of carbon have been previously shown to act as pressure cells under electron irradiation, driven by the self-compression of coherent layers upon the removal of atoms. Such nanoscale graphitic pressure cells were suggested to be interesting nano-laboratories for studying various in-situ pressure-induced phase transitions or chemical reactions.

Here we report that controlled irradiation of multiwalled carbon nanotubes can cause large pressure (up to 40GPa) buildup within the nanotube cores that can plastically deform, extrude, and break solid materials that are encapsulated inside the core [1]. The elastic and plastic deformation of nanometer-sized metal crystals inside carbon onions is monitored at an atomic scale by in-situ electron microscopy [2,3]. Compressive forces from graphitic shells lead to a slow but considerable deformation of encapsulated Au, Pt, W, and Mo crystals. Furthermore, a reaction between graphite and iron in the core of the carbon onions and growth of new carbon nanotubes inside host tubes were observed [4,5]. Thus, closed-shell carbon nanostructures such as carbon onions and nanotubes can be used as high-pressure deformation and reaction cells for deforming hard nanomaterials, modifying their properties, and investigating the behaviour of individual nanocrystals under high pressure.

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Open-ended, thin-walled carbon nanotubes filled with ferromagnetic nanowires: synthesis and applications

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As a group of nanoscale composites, carbon nanotubes (CNTs) filled with ferromagnetic metals (Fe, Co, Ni or their alloys) combine the magnetic property of metals with the electrical property of CNTs, exhibiting potential applications in diverse fields, for example in magnetic data storage, human tumor therapy, microwave absorption, probes for magnetic force microscopy and flat-panel display, etc. However, the manufacturing of ferromagnetic metal-filled CNTs with growth control still remains a real technical challenge. The sidewalls of CNTs are usually very thick (8~40 nm) and most of encapsulates exist in the form of particles or short rods (length <500 nm), which is almost no control at all. In addition, the synthesized CNTs are usually close-cap ended, which is not ideal for their field-emission performance.

In present work, a general strategy for in-situ synthesis of open-ended, thin-walled carbon nanotubes (CNTs) filled with long ferromagnetic (FeNi [1, 2], Fe-Co, FeCoNi, etc. [3]) nanowires is proposed. The key feature of this strategy is the introduction of Cl-contained benzene (e.g. trichlorobenzene) as carbon precursor. Size-dependent etching effect of Cl radicals on the sidewalls of CNTs is proved by theoretical calculations. As-prepared thin-walled FeNi-filled CNTs (FeNi-CNTs) show much lower turn-on field of 0.30 V/√56m (at 10 √56A/cm²) and lower threshold field of 0.65 V/√56m (at 1.0 mA/cm²) than those of thick-walled counterparts. Moreover, as-prepared thin-walled FeNi-CNTs show good field-emission stability at a low vacuum level (10⁻⁶ Torr). The enhanced field-emission performance can be attributed to a combined contribution of open-end tips, thinner sidewalls and metal nanowire fillings. When they were dispersed into epoxy resin to form microwave-absorption coatings, reflection loss exceeding -5 dB was obtained between 5~18 GHz for coating containing 1.3 wt % FeCo-filled CNTs. A minimum reflection loss value of -28.2 dB was achieved at 15.2

GHz in FeCoNi-CNTs/epoxy coating. The areal densities of coatings are only 2.35 kg/m² with coating thickness of 2.0 mm, which is favorable for the microwave-absorption applications requiring low density [3].

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Contribution D.05 - Tuesday, June 23

Application of Carbon Nanotubes in Nuclear, Particle and X-Ray Physics

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After the first consideration [1] of the possible use of carbon nanotubes in high energy and X-ray physics based on the unique properties of nanocrystals and bundles of carbon nanotubes, many theoretical and numerical works devoted to this problem have been published by Lyon-Moscow-Kharkov-Yerevan collaboration and other groups (see the review [2]). Experimental results on nanotube based detectors sensitive to UV [3] and IR [4] photons, as well as proposals [5] for the use of single nanotubes for beam particle monitoring and for construction of ionization counters for separate particles also are available. In this invited talk the physical principles of such applications are discussed, a review of the published works and construction of the corresponding devices and detectors are given.

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Use of Single Carbon Nanotubes for Beam Particle Monitoring and Detection of Separate Charged Particles

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The nanocrystals and bundles of carbon nanotubes can be used for various applications of high energy and X-ray physics [1]. In this work it is shown that due to unique physical properties, namely, high Young's Modulus and good electrical and thermal parameters, the single nanotubes also can help to solve many actual problems of beam particle monitoring and detection of separate particles if some difficulties connected with manipulation with already produced long nanotubes will be overcome. The physical principles, construction and advantages of nanotube beam monitors as well as of single wire and multiwire ionization counters measuring the ionization, coordinates and other parameters of separate high and low energy particles are discussed.

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Biomedical Applications of Carbon Nanotubes

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Biological applications of carbon nanotubes have been attracting a lot of attentions recently. In the past few years, we have studied the in vivo biodistribution, tumor targeting, long term fate and toxicity of functionalized single walled carbon nanotubes (SWNTs). We have uncovered that SWNTs with proper surface chemistry are biocompatible and non-toxic in vitro to cells. After intravenously administered into mice, SWNTs are accumulated in the reticuloendothelial systems

(RES) including liver and spleen, and slowly excreted via biliary pathway in feces without exhibiting obvious side effect. After those fundamental studies, for the first time we have shown that carbon nanotubes can be used as drug delivery vehicles for in vivo cancer treatment in mice xenograft tumor models. Moreover, the intrinsic optical properties such as resonance Raman scattering of SWNTs allow us to track and image them in vitro and in vivo. Multiplexed multi-color Raman imaging can be realized by using isotopically modified SWNTs. Taken together, carbon nanotubes are promising materials for future multimodality cancer therapy and imaging.

Contribution D.08 - Tuesday, June 23

Radial compression induced phenomena in single wall carbon nanotubes: the semiconductor-metal transition and the universal mechanical response

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Since the early 90's, the electronic and structural properties of single-wall carbon nanotubes (SWNTs) have been thoroughly investigated. Regarding deformation-induced properties, most of the attention has been given to axial deformations, even though several electromechanical effects have been observed on radially compressed SWNTs, such as the predicted [1] metal-insulator transition. We here report novel experimental and theoretical results on the mechanical [2] and electromechanical [3] response of SWNTs to radial compression.

First, we report [3] the direct experimental observation of the semiconductor/metal transition in SWNTs induced by compression with the tip of an atomic force microscope. This transition is probed via electric force microscopy by monitoring SWNT charge storage. Experimental data show that such charge storage is different for metallic and semiconducting SWNTs, with the latter presenting a strong dependence on the tip-SWNT force during injection. In the specific case of a semiconducting nanotube with a diameter of 1.7 nm, the tube becomes metallic

with an applied force per unit length of about 7 N/m, which causes a radial deformation that reduces the wall-to-wall separation to about 0.6 nm. This observation is well accounted for by ab initio calculations that indicate a semiconductor-metal transition at the same magnitude of radial compression as in the experiment.

We also report [2] the observation of a universal-type behavior of the mechanical response of SWNTs to radial compression. Specifically, we find that the quantity $Fd^{3/2}R^{-1/2}$, where F is the force applied by an AFM tip (with radius R) and d is the SWNT diameter, is a universal function of the compressive strain. Such universality is reproduced analytically in a model where the graphene bending modulus is the only fitting parameter. The application of the same model to the radial Young modulus E_r leads to a further universal-type behavior that explains the large variations of the SWNTs E_r reported in the literature. Finally, the implications of such universal-type behavior to nanometrology are briefly discussed.

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Contribution D.09 - Tuesday, June 23

Mechanics of hybrid carbon nanotubes - effect of the core filling

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Filling carbon nanotubes (CNTs) with materials as diverse as metal halides and biomolecules is a field that has matured considerably over the past 15 years. Today, the range of substances known to encapsulate within the empty tubular

space of CNTs is very broad indeed constituting a new class of materials denominated hybrid carbon nanotubes.

As recent studies demonstrate there is a measurable effect of the filling on the properties of the CNTs [1]. Hence, it is highly likely that an all new set of functional nanomaterials will result in the near future. Towards this, we have recently showed that the current conductance of Cu-filled carbon nanotubes can be manipulated to the point where these composite systems behave as rheostats [2]. Changes to the electrical behaviour may also potentiate the design of efficient nanodelivery devices [3]. In contrast to the electrical studies, the mechanics of hybrid CNTs have not been explored yet. With aim to integrate hybrid CNTs in nanoscaled devices it is desirable to know how these systems behave under external forces, such as compressive stress.

Here we present a pioneering study on the influence of the CNTs filling in the mechanical behaviour of carbon nanotubes [4]. The chosen system was a turbostratic carbon nanotube with Ga-doped ZnS encapsulated throughout its entire length. Using an integrated atomic force microscopy transmission electron microscopy technique it was possible to estimate the elastic modulus of the hybrid CNTs before and after the semiconducting-core release. It was found that, for this particular system, the core dominates the stiffness of the composite system.

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Contribution D.10 - Tuesday, June 23

The influence of the surface roughness of substrate on the

tribological behavior of carbon nanotubes coating

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The carbon nanotubes coating was deposited by Alcohol catalytic chemical vapor deposition (ACCVD) on top of WC-Co substrate of different roughness. The tribological properties were evaluated under standard fretting test at low humidity. The results show a dependence of coefficient of friction (COF) on the roughness of substrate.

Contribution D.11 - Tuesday, June 23

Mass sensor based on relative vibrations of walls of carbon nanotubes

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A new type of ultra high frequency nanoresonator based on the relative vibrations of the walls of carbon nanotubes is proposed. The resonator could be used for the detection of absolute mass of nano-objects with atomic resolution. The scheme of mass nanosensor is suggested. The resonance can be determined through registering a change in the gate-nanotube capacity, which depends on the amplitude of vibrations of the wall with the attached nano-object. The change in the capacity causes the change in the current through the nanotube that can be measured.

Density functional theory is used to compute the interaction energy of the walls of carbon nanotubes as a function of their relative position (see [1,2] for details of calculation technique). The computed interaction energy curves are fitted analytically and further exploited in the calculations of the frequencies of small relative axial and rotational vibrations of the walls for the set of double-walled carbon nanotubes (DWNT) with nonchiral commensurate walls. These frequencies are found to be in the range 70-700 GHz and do not depend on the length of the walls for nanoresonator with the vibrating wall which is shorter than fixed one. The shear strength for relative motion of walls is also calculated. Experimental measurements of calculated quantities using terahertz vibrational spectroscopy and atomic force microscopy techniques are suggested.

To estimate the sensitivity of mass detection by the proposed mass nanosensor and the quality factor of the resonance, microcanonical molecular dynamics simulations of the model resonator based on the (9,0)@(18,0) DWNT with the movable outer wall have been performed. The estimated average values of the resonator Q-factor are $Q=160$ at 77 K and $Q=540$ at 4.2 K, with the mass sensitivity of 4.5 and 1.3 carbon atoms at 77 K and at 4.2 K, respectively.

Recent advances in techniques for building of nanotube-based nanoelectomechanical systems are discussed.

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Contribution D.12 - Tuesday, June 23

Carbon nanotube based biomedical agents for heating, temperature sensing and drug delivery

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Due to their extraordinary physical and chemical properties carbon nanotubes (CNT) reveal a promising potential as biomedical agents for heating, temperature sensing and drug delivery on the cellular level. By filling the carbon nanotubes with tailored materials they can act as a chemically and mechanically stable nanocontainer. The carbon shells encapsulate the active material and protect it from wear and oxidation. Additional carbon is a perfect material for exohedral biofunctionalisation and so ideal for biomedical applications.

We describe the synthesis of CNT and the filling by different ways and show the structural and magnetic characterisation. In particular, the filling with magnetic materials offers the potential for hyperthermia applications while the insertion of NMR active substances allows the usage as markers and sensors. One example is the filling with CuI or AgCl, which exhibit a temperature dependent NMR signal so that nanoscaled contactless temperature sensors are realised. The potential of carbon nanotubes for biomedical applications is highlighted by hyperthermia studies which prove their applicability for local in-situ heating. In addition we have shown that a non-invasive temperature control by virtue of a carbon-wrapped nanoscaled thermometer. Also the filling with anti-cancer drugs is possible and the containers can be used for chemotherapy by drug-release at the cellular level. This will minimise adverse effects by decreasing the needed drug doses. Summarising these nanocontainers can act as magnetic nano-heaters, temperature sensors and drug-carrier systems for therapy and diagnosis at cellular level - with a focus on anti-tumour treatment.

Contribution D.13 - Tuesday, June 23

Synthesis of an MWNT/manganese oxide nanocomposite for use in insensitive nanothermite mixtures

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The classic thermite mixture, used e.g. for welding rails, is composed of Fe₂O₃ as an oxidant and Al powder as a reducing agent; the redox reaction creates large amount of heat and (in this case) liquid iron. By using nanostructured components

for a thermite mixture, the combustion velocity can be accelerated by a factor of 10,000 or more, close to the values of deflagrating explosives [1]. A variety of such nanothermites have been prepared in our laboratory in the past [2,3]. Some of these, especially nanostructured MnO_2/Al mixtures, have a very high friction sensitivity, making them dangerous to handle [3].

Enclosing manganese oxide inside carbon nanotubes reduces the sensitivity of such pyrotechnical mixtures while potentially keeping the high combustion rate and very low ignition delay. Here we present the synthesis of a multi-walled carbon nanotube/manganese oxide composite (MWNT/ MnO_x , $x \sim 1.62$) and the preparation of a nanothermite mixture made of this composite and aluminum nanoparticles (50 nm diameter) by physical mixing in a non-solvent (*n*-hexane). The nanotube composite is synthesized using an easy two-step method and is characterized by thermal analysis (DTA/TG), Raman spectroscopy, X-ray diffraction, and nitrogen adsorption (BET method). The impact sensitivity of this nanothermite (24.5 J) is found to be comparable to the classic nano- MnO_2/Al mixture (31.9 J [3]). However, its friction sensitivity is reduced to $> 360 \text{ N}$ (i.e. practically friction insensitive) while the MnO_2/Al nanothermite is extremely sensitive ($< 5 \text{ N}$). As predicted, the friction sensitivity is dramatically reduced by the physical separation of the reactive phases.

The velocities and ignition delays are measured by Time-Resolved Cinematography, i.e. by igniting compressed pellets with a CO_2 laser and recording the combustion using a high-speed camera.

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Temperature dependent resistance and infrared emission characteristics of carbon nanotube network films by inkjet printing

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We present the fabrication and characterization of temperature sensitive resistors using inkjet printed single-wall and multi-wall carbon nanotube network films.

By using inkjet printing process, very stable electrical properties can be achieved without preselection of nanotubes, even in the case of SWCNT, enabling a low cost fabrication of printed electronics such as touch panel and infrared sensor.

Centrifuged aqueous solutions of CNT with 0.5 wt.% density was used to achieve a stable drop ejection while avoiding nozzle clogging.

Single nozzle piezoelectric inkjet heads with 50 micron inner diameter were used to print resistor patterns with a size of 0.3 mm by 5 mm on Pyrex glass substrates up to 8 layers. The samples were annealed in a tube furnace with or without air at various temperatures.

Very high density network films of CNT were fabricated by repeated inkjet printing. All the samples show linear I-V curves and the conductance was almost proportional to the number of layers. The resistance decrease with the annealing temperature slightly. The most dramatic effect of annealing was a transition from negative temperature coefficient to positive one for the samples treated over 200 degree Celsius, depending on a relation between contact resistance and ohmic transport, which is useful for a various temperature sensing applications.

To test the thermal properties of the CNT network films, CNT patterns were printed on a porous silicon wafer covered with silicon oxide film. The surface tension of the CNT ink drops make a floating CNT network film, which enabling a very low thermal conductance to the substrate. The fast response mid-IR emission characteristics due to extremely low thermal mass of floating CNT structure were examined by nitrogen-cooled HgCdTe detector, suggesting the future application of high speed infrared source.

H ON CARBON NANOTUBES: ADSORPTION, KINETICS AND ELECTRONIC PROPERTIES

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Recent field ion microscopy studies evidence that hydrogen adatoms adsorbed on the surface of carbon nanotube (CNT) form hillock-like protrusions with height between 1 to 3 Å, which are interpreted as hydrogen nanoislands. This interpretation is supported by ab initio density functional calculations indicating that hydrogen adatoms on the nanotube surface have long ranged interaction with a positive binding energy. Interacting hydrogen atoms also create paired electronic states in the nanotube band gap [1], which is also in qualitative agreement with experimental observations. The goal here is the detailed study of hydrogen adatom clustering on carbon nanostructures using multiscale approach, which combines density functional calculations and Monte Carlo simulations.

In order to obtain the safe basis for the description of hydrogen diffusion and clusterization on the nanotube surface, we have calculated the potential energy surfaces (PES) for a hydrogen atom and for two interacting hydrogen atoms on carbon nanotube. Also the effect of the curvature to adsorption and desorption energies for hydrogen atom and dissociation of hydrogen molecule is investigated. On applying the obtained values for kinetic Monte Carlo simulations of chemisorbed hydrogen annealing, a noticeable influence of the annealing conditions on cluster sizes, shapes and relative populations has been revealed [2], which opens a possibility for the control of hydrogen clusterization kinetics. The effect on CNT electronic structure and raman spectra from hydrogen dimers and trimers most frequently met in KMC simulations is discussed.

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Contribution D.16 - Tuesday, June 23

Structural studies of carbon nanohorns by neutron and X-ray diffraction

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The structure of carbon nanohorns produced by laser ablation at room temperature without a metal catalyst [1] has been studied using the neutron and X-ray diffraction techniques and the molecular dynamics (MD) method. The neutron diffraction measurements were carried out on the GEM (GEneral Materials diffractometer) at the Rutherford Appleton Laboratory. The scattering data were measured up to the scattering vector $Q_{\max}=30 \text{ \AA}^{-1}$ ($Q=4\pi\sin\theta/\lambda$, where 2θ is the scattering angle and λ is the wavelength). The X-ray diffraction data were recorded using a laboratory diffractometer with the monochromatized Ag radiation up to $Q_{\max}=22 \text{ \AA}^{-1}$. The collected diffraction data have been converted to a real space representation in the form of the pair correlation function via the Fourier transform. The structural model consisting of a nanocone with the cone angle approximately 20° and a single-wall carbon nanotube of about 35 nm in length and 2 nm, 2.5 nm and 3 nm in diameter has been computer generated starting from a single graphite layer. The presence of the defects in the form of pentagon-heptagon pairs via the Stone-Wales mechanism has been considered [2]. Then this model has been relaxed using the MD method with the reactive empirical bond order potential [3]

for carbon-carbon interaction and the Lennard-Jones potential with parameters for inter-layer interactions [4]. Correctness of a such constructed model has been verified by comparison of the simulations and the experimental data in both real and reciprocal space.

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Contribution E.01 - Thursday, June 24

High-density Arrays of Carbon Nanotube and Graphene Devices: Directed Assembly and Rapid Characterization

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In the recent years, significant strides have been made in demonstrating unique and high-performance functionality in single-walled carbon-nanotube (SWCNT) and graphene electronic devices. However, high-density directed assembly, integration and rapid characterization of a large number of devices for statistical analysis remains major challenges. Here, I present our recent developments in our group towards achieving these goals.

First, I will discuss the fabrication of high-density arrays of single-chirality SWCNT [1] and of graphene [2] devices. Recently, we have demonstrated that dielectrophoresis can be used to fabricate high-density arrays of SWCNT devices, and that the process is self limiting to one nanotube per device. [3] Single-chirality nanotube suspensions are obtained by selective polymer wrapping and density gradient ultracentrifugation. Graphene solutions are made by exfoliating graphite in aqueous and various organic solvents. The yield and quality of nanotube and graphene devices from a variety of suspensions will be compared. The

arrays are characterized by spatial Raman and photoluminescence maps and electronic transport measurements.

In the second part, I will present Voltage-Contrast Scanning Electron Microscopy (VC SEM) as a new technique for the rapid, parallel and visual electronic characterization of carbon nanotube devices and arrays. This technique is based on the fact that the secondary electron yield depends on surface potentials. VC-SEM is demonstrated to distinguish metallic and semiconducting nanotubes in the SEM, [4] and the mechanism of contrast evolution is discussed. Furthermore, the contrast profile along a nanotube changes abruptly in the presence of defects, and this can be used to locate and characterize them. VC-SEM is demonstrated in the characterization of typical defects, [5] such as Stone-Wales defects, high-current breakdown, electron-beam induced metal-insulator transition and charge-injection into the dielectric substrate.

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Contribution E.02 - Thursday, June 24

Measurements on quantum capacitance of individual single walled carbon nanotubes

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We report measurements of the quantum capacitance of individual semiconducting and small band gap single walled carbon nanotubes (SWNTs). The ob-

served quantum capacitance, 82 aF/nm for a semiconducting SWNT with chiral index (16,8) and 10.3 aF/nm for a small band gap SWNT upon Fermi level lying at the first subband are remarkably smaller than those originating from the density of states. We attribute the discrepancy to a strong electron correlation in SWNTs and derive the Luttinger parameter g of 0.250.3 for the (16,8) SWNT and of 0.32 for a small band gap SWNT.

Contribution E.03 - Thursday, June 24

Electronic and Transport Properties of Single and Multiwall Carbon Nanotubes under Mechanical Deformations

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Carbon nanotubes (CNTs) can be metallic or semiconductors depending simply on geometric characteristics. This peculiar electronic behavior, combined with high mechanical strength, make them potential building blocks of a new nano-electronic technology. High resolution images of CNTs often disclose structural deformations such as bent, twisted, or collapsed tubes. These deformations break the tube symmetry, and a change in their electronic properties should result.

A computationally effective mixed finite element-tight-binding approach able to simulate the electromechanical behavior of single and multiwall nanotubes used in nano-electronic devices is presented. The finite element (FE) computes the evolution of atomic coordinates with deformation and provides these coordinates to a tight-binding (TB) code, enabling computation and updating of the electrical conductivity. The TB code is engineered to realize dramatic computational savings in calculating deformation-induced changes in electrical transport properties of the nanotubes. The FE-TB computational approach is successfully validated in a simulation of laboratory experiments which had measured the changes in electrical conductivity of a multiwall carbon nanotube during mechanical deformation.

Contribution E.04 - Thursday, June 24

In-situ TEM study on electric and mass transport of a copper nano-rod encapsulated in a carbon nanotube

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One-dimensional structures such as metal nanowires and nano-rods are attracting considerable attention because of their potential applications to building blocks for electronic devices. Hybridization of metal nano-structures and carbon nanotubes (CNTs) is a promising method to provide a new class of materials with synergistic functions of individual nano-materials. Here, we investigated the electric property and structural change of the individual nanotube encapsulating the copper (Cu) nano-rod by in-situ transmission electron microscopy (TEM).

Cu filled CNTs, which were synthesized by the laser vaporization of graphite containing copper, were dispersed on a TEM grid. A tungsten needle was made contact to individual CNTs protruding from the copper plate inside a TEM. Electric voltage was applied between the ends of a Cu nano-rod encapsulated in CNT, and the structural change was observed with a TV camera.

The diameter and the length of the Cu filled CNT were 18 nm and 256 nm, respectively. The thickness of the graphite layer was about 1 nm, consisting of several layers of graphite. Some spherical Cu particles adhered to the CNTs. The electric voltage was applied between the two ends of the CNT inside the TEM. At 1.4 V, the current increased to 10 μ A, corresponding to a current density of 4.0×10^6 A/cm², and at the same time the Cu nano-rod started to move to an end of CNT, leaving the CNT sheath. After the shrinkage of the Cu nano-rod, an empty CNT was left. From the variation in the total resistances measured for the different lengths of the Cu nano-rod, electric resistivities of the CNT and the Cu nano-rod were measured to be 3.0×10^{-5} Ω m and 1.2×10^{-4} Ω m, respectively. The resistivity of the CNT is comparable to that of graphite, whereas the resistivity of the Cu nano-rod is much higher than that of bulk Cu. A probable cause of the high resistivity of the Cu nano-rod is scattering of carriers by its surface.

The direction of the Cu transport seems to depend on the direction in which the debris Cu particles adhered to the CNT rather than the direction of a current flow.

Defective carbon nanotubes: magnetism, spin transport and gas sensing applications.

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Carbon nanotubes (CNTs) are renowned in the scientific community for being both a playground for studying fundamental physical properties and for applications in, to mention a few, electronic, spintronic and gas sensing technologies. However, despite the progresses in growth techniques, CNTs always exhibit structural defects [1] and their electronic and transport properties will be affected accordingly [2]. In addition, the presence of defects in carbon-based nanostructures has been seen as source of magnetism [3]. Hence, mastering the physics underlying defected CNTs is crucial not only to model realistic systems but also to design new devices.

The spin-polarized electron transport properties of carbon nanotubes with vacancies are investigated using first principles and non-equilibrium Green's function techniques [4]. Carbon atoms with unsaturated bonds are found to behave as quasi-localized magnetic impurities, coupled by long range interactions. The magnetism of carbon nanotubes with reconstructed mono- and tri-vacancies results in spin dependent conductances and, hence, can be exploited in spintronic devices such as nano-spin valves.

Clarified the properties of CNTs with vacancies, the sensing ability of defected CNTs towards several molecules (NO_2 , NH_3 , CO , CO_2 , H_2O) has also been investigated *ab initio*. Since the adsorption/desorption of molecules induces modulations on the electrical conductivity of the tube, quantum conductances of the CNT-based sensors are predicted, finding that defective nanotubes are sensitive to NO_2 , NH_3 and CO , while molecular selectivity is provided by the nature of the charge transfer.

This work is supported by the project "Nano2Hybrids" (EC-STREP-033311).

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Contribution E.06 - Thursday, June 24

Magnetism and electron transport in metal decorated carbon nanotubes

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First principles Density Functional Theory (DFT) and Non Equilibrium Greens Function (NEGF) methods have been used to investigate the magnetic and electronic transport properties of carbon nanotubes (CNTs) decorated with metallic nanoclusters.

CNTs can be thought as one-dimensional conductors and, as such, offer the opportunity of studying fundamental issues in electronic transport at the nanoscale. Metallic nanoclusters exhibit peculiar structural, electronic, and magnetic properties due to their finite size. In particular, small clusters of magnetic (as, for instance, Ni [1]) and non magnetic (as Au [2]) elements can have a net magnetic moment whose magnitude depends on the cluster size. Hence, decorating carbon nanotubes with nanometer-size metallic clusters can lead to nanomaterials with interesting magnetic properties, such as a spin-dependent conductance [3].

In addition, CNTs decorated with metal clusters have been recently fabricated [4] and call for a theoretical investigation to unveil their fundamental properties and investigate possible applications in spintronic devices as nanomaterials with magnetic properties tunable with the cluster size.

This work is supported by the project “Nano2Hybrids” (EC-STREP-033311).

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Contribution E.07 - Thursday, June 24

Femtosecond laser patterned CNT for field emission applications

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The CNT array was fabricated by using a femto-second pulse laser based machining. This technique allows pattern carbon nanotubes without involving the conventional lithography methods. The field emission (FE) characteristics of as-fabricated CNT array showed the high current density of 5.74 A/cm^2 , the low turn-on electric field was $0.76 \text{ V}/\mu\text{m}$ (the respective current density of 1 mA/cm^2), and the emission stability was tested until 30 hrs without any degradation and damage. In this report, we present the alternative approach of making CNT-array on high doped silicon substrates which is accessible to make electron emitting sources.

Contribution E.08 - Thursday, June 24

Efficient Field Emission from Line-Patterned Carbon Nanotube Cold Cathodes

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Carbon nanotubes (CNTs) are expected as electron emitters to be applied for field emission (FE) displays. Single-, double- and thin-walled CNTs can be potentially used as emitters to lower the driving voltage. Here high density implementation of emitters is necessary to ensure emission uniformity and lifetime. We proposed the triode-type 1D-Array of single-walled CNT (SWCNT) emitters prepared through a quick CVD process for 5-15 seconds [1]. A low driving voltage and practical emission uniformity were demonstrated, however optimized cathode configurations and emitter morphologies to efficiently extract electrons have not yet been obtained. We report excellent FE properties and importance of emitter morphologies and numbers revealed for the renewed trench configurations.

An assembly of line-patterned micro-trenches (slit width: $0.8\ \mu\text{m}$, spacing: $10\ \mu\text{m}$, patterned area: $2\ \text{mm} \times 2\ \text{mm}$) was fabricated through electron-beam lithography. An Al_2O_3 underlayer ($10\ \text{nm}$) was then sputter-deposited through the gate slits. The Al_2O_3 on a resist/gate layer was removed by a subsequent lift-off process. A Co catalytic layer was next deposited on the substrates. The gate slits dilute deposition flux of sputtered Co, and therefore a gradient thickness profile of the Co catalytic layer and a uniform Co layer are formed on the cathode and on the gate, respectively. According to the combinatorial searching for catalytic/supporting material compositions [2], a thickness distribution with a peak value of $1.6\ \text{nm}$ on the cathode corresponding to a uniform thickness of $8.5\ \text{nm}$ on the gate gives a rapid SWCNT growth only in the trenches. Thermal C_2H_2 -CVD was carried out for 5-300 sec at $1073\ \text{K}$.

SWCNTs were selectively implemented on the cathode lines in the trenches. Excellent FE properties current densities (J_a : recorded at anode) of $1\ \mu\text{A}/\text{cm}^2$, $10\ \text{mA}/\text{cm}^2$ and $110\ \text{mA}/\text{cm}^2$ at the gate voltages (V_g) of 16, 25 and 37 V, respectively, were recorded. ΔV_g to gain 1:10,000 contrast of J_a was as low as 9 V, indicating very low operating voltage. Degradation of the FE properties is settled during continuous operation up to 7 hours in pulse mode ($V_g = 25\ \text{V}$, 1/2-duty, 100 Hz). Not only a large number of emission sites but also an optimal combination of trench structures and emitter morphologies are crucial to pull out the full FE potential of CNTs.

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Chemically Purified DNA-Single Walled Carbon Nanotube Hybrids: Controllable Redox Properties with Hydrogen Peroxide

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We report the controllable redox properties of chemically purified ssDNA-single-walled carbon nanotube (SWNT) hybrids with a biologically important oxidant, hydrogen peroxide, by monitoring the unique near infrared spectral intensity of SWNTs. Compared with the suspensions before separation, the purified SWNT suspensions become inert with hydrogen peroxide which may serve as a platform for further chemical manipulation. In the presence of thiocyanate ions, the reaction of SWNTs with hydrogen peroxide is initiated and accelerated at the earlier reaction stage, accompanied with the near infrared spectral suppression. At the later stage, the suppressed spectral intensity is recovered overtime. The thiocyanate ions may work as a mediator being able to control the reaction rate as well as the tunable properties of the reaction. The tunable redox reaction of SWNTs and hydrogen peroxide mediated by thiocyanate ions may offer a new optical sensing scheme for continuously monitoring hydrogen peroxide concentrations.

Semiconducting single wall carbon nanotubes investigated by photoconductivity and electromodulation spectroscopy

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Using semiconducting single wall carbon nanotubes with well defined chiral index (n,m), the photo-carrier generation mechanisms (essential in photoconductor and photovoltaic devices) and the Stark effects (essential in non-linear optical and electro-optical effects) have been investigated by photoconductivity and electro-modulation spectroscopy. This achievement was made possible, because very recently, we have developed a technique which selectively extract semiconducting SWNT with a limited extent of chiral indexes without detectable traces of m-SWNT, from HiPCO or CoMoCat samples using polyfluorene as an extracting agent assisted by sonication and ultracentrifugation techniques^{1,2}.

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Contribution E.11 - Thursday, June 24

Optical Spectroscopy Studies on Modified Optical Properties of Single- and Double-Walled Carbon Nanotubes

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Since the discovery of band gap photoluminescence (PL) from isolated single walled carbon nanotubes (SWNTs), PL maps have been widely utilized for

determining the relative (n, m) distribution of semiconducting SWNTs. The high sensitivity of PL in SWNT systems is very useful in sensing applications. However, carbon nanotube defects or functional groups on the sidewalls, of catalytically grown SWNTs created during oxidative purification processes, quench significantly the PL intensity.

In this study, we examined the changes in the optical properties of single- and double-walled carbon nanotubes which were consecutively modified by chemical treatments (e.g., oxidation, fluorination). We believe that the strong and stable PL signal from the inner tubes of DWNTs originates from their coaxial structures (or from the shielding effect of their outer tubes).

Contribution E.12 - Thursday, June 24

Observation of Exciton-Phonon Sideband in Individual Metallic Single-Walled Carbon Nanotubes

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Single-walled carbon nanotubes (SWCNTs) are quasi-one-dimensional systems with poor Coulomb screening and enhanced electron-phonon interaction, and are good candidates for excitons and exciton-phonon couplings in metallic state. Back scattering reflection experiments are performed on individual metallic SWCNTs. An exciton-phonon sideband separated by 0.19 eV from the first optical transition peak is observed in a metallic SWCNT of chiral index (13,10), which provides clear evidences of excitons in metallic SWCNTs. A static dielectric constant of 10 is estimated from the reflectance spectrum.

Contribution E.13 - Thursday, June 24

Dissipation of Excited Carriers from Semiconducting to Metallic Carbon Nanotubes: Time-Dependent Density Functional Calculations

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Aggregation of carbon nanotubes into bundles quenches the fluorescence which was attributed as excited-carrier dissipation through metallic nanotubes within the bundle [1]. However, no one knows how the carrier-transfer occurs through inter-wall spacing of 3.4 Å, where no covalent-bond networks exist. Indeed, there is no direct measurement of the carrier transfer process.

To demonstrate and to visualize the dissipation process of excited carriers in nanotube bundles, we performed ab initio calculations for electron-ion dynamics [2] using time-dependent density functional theory. This method successfully showed hot-carrier dynamics in an isolated carbon nanotube [3].

In the present calculations, the semiconducting (8,0) and metallic (9,0) nanotubes are placed in the same unit cell with inter-wall distance 3.4 Å. Throughout the molecular dynamics simulations at room temperature, we found that the excited states (E22) in the (8,0) nanotube sometimes hybridize to those of the (9,0) nanotube. The hybridization suggests easy dissipation of excited carriers through the metallic nanotube. In this presentation, we will present detailed dynamics of the carrier dissipation.

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Contribution E.14 - Thursday, June 24

Energetic Properties and Work function of K Intercalated Carbon Nanotubes Tip: Applications to Field-Emission.

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The knowledge of the work function energy plays a highly important role in an application of carbon nanotube for field emission devices. In this study, we therefore calculated the interaction energy and the work function as defined at mid-gap of between HOMO and LUMO energy of the K intercalated onto the carbon nanotubes tip (SWNTs) by using density functional theory (DFT). By using zigzag tube 2 unit cells, the tube diameter was $n = 9$. The intercalation of K at the center of tube through the nanotube tip of SWNTs. It was found that the work function of K at the exterior is higher than the interior of nanotube tip and K prefer to absorb onto interior more than exterior. The work function of the pristine carbon nanotubes tip (SWNTs) can reduce work function by intercalating K in both side wall of SWNT.

Contribution F.01 - Thursday, June 24

A COMPUTATIONAL STUDY ON THERMAL CONDUCTIVITY OF CARBON NANOTUBE DISPERSED BIOLOGICAL NANOFLUIDS AND SUSPENSIONS

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A computational model, based on the random movement of Brownian thermal walkers, has been developed to predict the effective thermal conductivity of an

idealized biological fluid and of suspensions containing single-walled carbon nanotubes (SWNTs). Thermal death of cancerous cells may be induced by radiating SWNTs selectively attached via functionalization to the targeted cells. A distribution of SWNTs inside cancerous cells, on their surface, or in the inter-cellular fluid may occur during this treatment process. The effects of the SWNT aspect ratio, weight fraction, and thermal resistance at the interface between the SWNTs and their surroundings were incorporated to make predictions that are required for developing an overall approach to cancerous cell targeting. The developed model was also applied to predict the thermal properties of SWNT dispersed in aqueous and oil suspensions. The dependence of the effective thermal conductivity on the temperature for aqueous suspensions was also investigated.

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Contribution F.02 - Thursday, June 24

Correlation between Resistance Fluctuations and Temperature Dependence of Conductivity in Graphene

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It is known that monolayer graphene has an extraordinarily high intrinsic mobility of the charge carriers. Important complications are the presence of mobile scattering centres that strongly modify charge transport, and the presence of strong mesoscopic conductance fluctuations that, in graphene, persist to relatively high temperatures. We investigate the surprisingly varied changes in resistance that we find in graphene flakes as temperature is lowered below 70 K. We propose that

these changes in $R(T)$ arise from the temperature dependence of the phase coherence length of scattered electron waves that causes the resistance fluctuations observed at low temperatures vanish as the temperature rises up to 70 K. Using the field effect transistor configuration, we verify this explanation in detail from measurements of $R(T)$ at constant gate voltages tuned to particular features of the resistance fluctuations that correspond either to the constructive or to the destructive electron wave interference. The proposed interpretation was verified for the low charge carrier densities close to the charge neutrality point as well as for the high electron and hole density regions far from the neutrality point. The $R(T)$ were fitted by two different models taking into account firstly electron-phonon scattering for the high carrier densities $R(T)$ and secondly activation of charge carriers in the case low carrier densities $R(T)$.

Contribution F.03 - Thursday, June 24

Electron-phonon coupling in graphene layers investigated by angle-resolved photoemission and inelastic x-ray scattering experiments

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We propose graphite intercalation compounds (GICs) as a material system with precisely the same electronic properties as doped few layer graphene[1,2].

Despite the fact that GICs have been around for the last four decades, this fact has gone unnoticed so far. Especially, we focus on the electronic energy bands of KC8 which corresponds to a doped graphene monolayer [2]. We provide extensive evidence for this claim employing a combined angle-resolved photoemission (ARPES) and theory approach including electron-electron correlation on a GW level. We observe a strong kink in the quasiparticle dispersion at 166meV highlighting electron-phonon coupling to an in-plane transversal optical phonon. These results are key for understanding, both, the unique electronic properties of doped graphene layers and superconductivity in KC8 and are an elegant way to circumvent the substrate interaction [3].

Based on our ARPES data we provide a new set of tight-binding (TB) parameters for efficient calculation on the quasiparticle dispersion in pristine and doped few-layer graphene and graphite including electron-electron correlations[4]. Within a tight-binding picture we investigate the family pattern of few layer graphenes and examine the transition to graphite.

Finally, we present inelastic x-ray scattering (IXS) measurements. The kink energy in the quasiparticle dispersion is compared to IXS data and is in good agreement to an observed Kohn anomaly for the TO phonon branch at K point. This reflects, that electron phonon interaction can indeed be seen in both the quasiparticle and phonon dispersion relation by ARPES and IXS, respectively.

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Contribution F.04 - Thursday, June 24

Motion and Manipulation of Suspended Single-Walled Carbon Nanotubes in Solution

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We have developed an optoelectronic imaging system which combines nanotube transistors with optical trapping techniques and the scanning photocurrent microscopy to investigate the motion of suspended single-walled carbon nanotubes in solution. This setup enables us to study the movement of nanotubes by monitoring their photocurrent images and to measure their thermal fluctuations through observing the movement of microbeads that are tightly attached to nanotubes by single-stranded DNA. By analyzing their thermal fluctuations, we are able to obtain the torsional and transversal stiffness of nanotubes and then calculate their diameters. We can also manipulate their motions by using an optical trap to pull on microbeads attached to nanotubes.

Contribution F.05 - Thursday, June 24

High speed carbon nanotube memory elements

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Single-walled carbon nanotube field-effect transistors (CNT-FETs) are demonstrated to have impressive device parameters. They are extremely fast having a transit frequency as high as 50 GHz [1] and have high sensitivity in monitoring single-electron tunneling events between a gold particle and a nearby nanotube [2]. These CNT-FETs display often some degree of hysteresis in their transfer characteristics. For a transistor this is an unwanted attribute but it opens up new possible applications. By utilizing this hysteresis, CNT-FETs can be used as a memory element. The insulator film between the gate and CNT has here a crucial influence on the operation of the CNT-FET [3]. For an effective capacitive coupling between the CNT and the gate electrode, a thin and dielectrically strong film is required. On the other hand, in order to achieve the desired hysteretic behavior for memory operation, the gate-nanotube coupling has to include charge traps within the gate insulator or at some interface in the system that can be filled or

emptied with charges from the CNT.

Here we will present the first results on a first high performance charge trap CNT memory element having HfO₂ gate dielectric and operation speed below a microsecond regime [4]. We will also show results on other device parameters like endurance under continuous operation and retention time. A simple model is constructed to show that fast charging and recharging of HfO₂ defects by charge carriers from the CNT is likely.

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Contribution F.06 - Thursday, June 24

Lithography-free dry fabrication of carbon nanotube field-effect transistors

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Recently, we have developed and investigated a low-cost method to manufacture carbon nanotube field-effect transistors (CNT FETs). The method is based on

aerosol technology for single-walled CNTs synthesis and deposition. The deposition of CNTs onto the substrate in the form of a network occurs at room temperature instantaneously after the CNT growth. Time-consuming solution-based CNT network (CNTN) preparation steps, capable to degrade the CNT pristine qualities, are eliminated. The density of a CNTN is controlled by varying the deposition time. The method enables scalable and low-cost manufacturing of high-performance thin film transistors on various substrates including heat-intolerant plastic materials [1, 2]. However, this method still requires utilizing photolithographic processes.

Here we demonstrate a novel method for all-dry lithography-free fabrication of CNTN FETs. This technique is based on using a shadow mask for direct dry deposition of CNTs onto a substrate from the aerosol synthesis reactor and subsequently defining metal electrodes using e-beam evaporator. Dielectric layers are prepared by atomic layer deposition (ALD) technique. The mask during the whole fabrication process remains intact on the substrate, allowing precise electrode-CNTN channel alignment. Lithographic processes are removed in the fabrication procedure, allowing all-dry simple manufacturing technique. Shadow-mask fabrication peculiarities connected with CNTN deposition through the mask will be discussed. Electrical measurement results of as-fabricated CNTN FETs will be presented.

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Contribution F.07 - Thursday, June 24

Atomic layer deposition on single-walled carbon nanotubes for device application

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Carbon nanotubes (CNTs) are between the most promising materials for electronics. Devices based both on individual nanotubes and on carbon nanotube networks (CNTN) have been proposed. CNTN retains many of interesting properties of individual single-walled nanotubes (SWNTs) while providing the processing capabilities of mass fabrication methods. Atomic layer deposition (ALD) seems to be one of the best techniques for thin and conformal coating of CNTs, especially on polymer substrates, where process temperatures are limited. On the other hand, the ALD process on inert CNT surface is rather complicated [1].

In this work we investigate the growth of ALD aluminum oxide layer on CNTs, both on individual nanotubes and on their bundles. The samples were obtained by direct dry deposition of SWNTs. This new technique is very attractive because it allows deposition of CNTN on different substrates at room temperature [2]. The ALD growth (from one nanometer till tens of nanometers thick layers) on nanotubes was monitored by transmission electron microscopy (TEM). ALD process was performed at different temperatures (80°C and 200°C), and using different precursor for oxidation (water and ozone). Differences between the coating of individual CNTs and their bundles have been obtained, what can be attributed to the different surface activation. ALD technique was used for the passivation of fabricated CNTN transistors and gate oxide formation for top-gated field-effect transistors. The obtained results confirm great potential of ALD technique in CNT based electronics.

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Contribution F.08 - Thursday, June 24

Modifying the Electrical and Optical Properties of Organic Thin Film Transistors by adding the Carbon Nanotubes Inside the Channel Material

Hua-lun Tsai, Jeng-Hua Wei, Ting-Chun Huang

To fabricate the flexible solar cells, the many organic-base materials are proposed in the literature and the combination of P3HT and C60 derivate PCBM is the most popular active material. However, because this material has a lower mobility and the channel length of organic devices which fabricated by the low-cost print technology is long, the electrical properties and optical responses of OTFTs are still poor. In this report, we add some CNT ropes inside the active layer and it will reduce the effective channel length of the OTFTs by optimizing the ratio between P3HT, PCBM and CNTs.

In our study, the device is fabricated on the PET substrate and the process temperature is less than 100oC. Considering the safety issue, we chose the toluene as the solvent of the P3HT, PCBM and CNTs and the optimal ratio between P3HT, PCBM and CNTs is the 4:2:1. To collect the information of the devices current flow, we design a stack-type, double source/drain electrodes in the device. In one OTFT, we can record the I-V curves of OTFTs with the top-contact or bottom-contact configuration. For the optical response, the current changes of the devices with vertical and lateral structures are also recorded. After studying these data thoroughly, we can find the effect of the CNT ropes in the organic-base devices.

Contribution F.09 - Thursday, June 24

Using of carbon nanotube and the aqua of nano silver to adopt the manufacturing process of the whole aqueous solution to manufacture organic thin film transistor on the flex

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In this paper, we report an all-soluble process for the carbon nanotube organic thin film transistors (CNT-OTFTs) by combining the liquid-phase-deposition (LPD) oxide, soluble CNTs and nano-metal particles. First, the CNT powders are dissolved in the sodium sulfate (SDS) and water by the ultrasonic mix. Then the CNT films are coated by spin-on process and baked in 90oC. In this report, the

CNT layers are used as the active channel and metal electrodes. In some devices, we use the silver as the electrodes. For the silver electrodes, the nano silver particles are dissolved in the ethylene glycol in the different ratios. In order to avoid the organic solvent damage the underlying layer and suppress the leakage current in the OTFTs, we use a water-based LPD silicon oxide as the gate insulator and passivation layer. This oxide is deposited at 50°C by using the hydrofluosilicic acid (H₂SiF₂) and water.

In this report, the top-contact CNT-OTFTs are completed without using any vacuum process. Before coating the CNT films as the channel layer and electrodes, the CNT solution is filtered and the undissolved CNT powders are removed. After completing the CNT OTFTs, the electrical properties of these devices are measured by the Agilent 4156C in the air. Due to both the CNTs and silicon oxide are air-stable materials, the devices by using new process show the good characteristics.

Contribution F.10 - Thursday, June 24

Individual 1D nano-object characterizations in GHz range using in-situ high impedance measurement set-up

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CNT or metallic and semi conducting nanowires present high impedance, the observation of individual nano-object behavior in GHz is thus crucial but represents a serious experimental challenge.[1,2] This presentation describes a device to characterize high frequency 1 D nano-object. The measurement technique is compared to standard technique with 50 Ω Vector Network Analyzer (VNA). It allows the reduction of mismatch between the nano-object impedance and the VNA impedance, and consequently the reduction of the measurement error.[3] The measurement method has been validated on metallic SWNT, and expanded to Si nanowires. The major results obtained will be presented and discussed. As an example, individual metallic carbon nanotube is characterized up to 7 GHz with

unprecedented precision and an equivalent circuit is extracted without any fitting parameter.

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Contribution F.11 - Thursday, June 24

Superconductivity in boron-doped carbon-nanotubes

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Superconductivity (SC) in carbon nanotubes (CNTs) is attracting considerable attention from the viewpoints of (1) electron correlation in one-dimensional (1D) SC, (2) carbon-based new-superconductor family;(CaC₆ and boron-doped diamond), and (3) realization for high-T_c SC due to high-phonon frequency of carbon atoms and strong electron-phonon interaction in the thin tube structure. Previously, we reported on SC in the arrays of multi-walled CNTs (MWNTs) with the world-highest T_c = 12K and its correlation with 1D electron correlation [1]. After then, many theories for the CNT-SC have been proposed; e.g., 1.Carrier doping effect in MWNTs and 1D electron correlation [2] and 2.Carrier doping effect in semiconducting single-walled CNTs (SWNTs) [3].

Here, we have had significant progress in the experiments after reporting Ref.[1] e.g., (1) confirmation of possible Meissner effect [4], (2) Observation of interplay of SC and 1D electron correlation (Tomonaga-Luttinger liquid states) [5], (3) Confirmation of presence of boron (B) in the MWNTs by NMR [6]. In particular, the third issue for B-doping was crucial for controlling the SC.

In the talk, I will show SC (Meissner effect) found in highly-homogeneous thin films consisting of B-doped SWNTs [7]. I show that B-doping above concentration of 4 atomic % destroys the SWNTs and reveal that only very small

B-concentration (< 1.5 atomic %) can lead to appearance of evident SC because of the better alignment of Fermi level to a van Hove singularity in the electronic density of states [7]. I will also show finding of pressure-induced TC up to 19K in films with much higher density of dissolved B-SWNTs (i.e., Buckypaper).

SC in carrier-doped CNTs is promising and will shed light to study of novel type 1D SC. It could lead to higher T_c up to 40K by further optimization of doping condition.

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Contribution F.12 - Thursday, June 24

The Alignment Growth of Carbon Nanotubes on Inconel Sheets using Hot Filament Chemical Vapor Deposition

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Vertically aligned carbon nanotubes (CNTs) are of great interest in applications such as electron-field emitters in panel display, scanning probe microscope tips, biological probes, and interconnect for nanoelectronics. In order to achieve the aligned growth of CNTs, it is essential to fully understand the alignment mechanism. In this work, the effect of bias voltage and substrate surface roughness on the growth of vertically aligned CNTs on Inconel sheets without addition

of catalyst was investigated using hot filament chemical vapor deposition in a gas mixture of methane and hydrogen. Well aligned CNTs have been synthesized by apply bias between the substrate hold and the filament. The results show that CNTs grown under negative bias display better alignment than the ones under positive bias. Bias of -500 V generates the best alignment. It has observed that at the early growth stage, aligned and non-aligned CNTs are growing simultaneously on the unscratched sheets whereas only aligned CNTs are growing on the scratched sheets. The results indicate that tip growth is not necessary for the electric field to align the CNTs, and larger catalyst particles created by scratching before the heat treatment can induce in the alignment of CNTs at the early growth stage. In addition, tree-like CNT bundles grown on the scratched substrates exhibit better field electron emission performances than dense carbon nanotube forest grown on the unscratched substrates due to the reduced screen effect.

Contribution F.13 - Thursday, June 24

Chemical reactivity and magnetism of graphene

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The basic problem of weak interaction between odd electrons in graphene is considered within the framework of broken spin-symmetry single-determinant approach. The modern implementations of the approach in the form of either unrestricted Hartree-Fock scheme (UBS HF) or spin-polarized DFT (UBS DFT) were discussed with particular attention to the applicability of spin-contaminated solutions of both techniques for the description of electronic properties of graphene. The UBS DFT applications generally reveal the open-shell character of the singlet state of the object and manifest an extra spin density concentrated on zigzag edge atoms (see [1] and references therein). Similarly, the current study shows that UBS HF approach supports these findings but exhibits the extra spin density not only on zigzag edge atoms but on all atoms of the sheet. This very peculiarity permits to quantitatively describe the odd electron behavior via both enhanced chemical reactivity and magnetism. The former is presented in terms of a quantified atomic chemical susceptibility that is homogeneously distributed over all nonedge inner

atoms with the value similar to that of fullerenes and CNTs sidewalls and is twice or five times more on zigzag edge atoms depending on if those are either terminated (by hydrogen) or empty. Armchair edge atoms 4 times prevail over inner ones only in the absence of chemical termination. Magnetic response of graphene sheets is provided by a collective action of all odd electrons and is size-dependent. The relative magnetic coupling constant J decreases when the sheet size increases and J approaches the limit value of 10^{-2} - 10^{-3} kcal/mol, needed for the object magnetization to be recoded, when the sheet size is of a few nm that is well consistent with experimental findings [2].

The explanation suggested by the UBS HF approach seems quite reasonable. A common view on both chemical reactivity and magnetism of graphene, physically clear and transparent, witnesses the approach internal self-consistency and exhibits its high ability to quantitatively describe practically important consequences of weak interaction between odd electrons. The statement is well supported by a deep coherency of the obtained UBS HF results with those followed from the application of many-body CI calculation schemes to acenes [3] and graphene [4].

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Contribution F.14 - Thursday, June 24

Broken spin-symmetry HF and DFT approaches. A comparative analysis for nanocarbons

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The quantum-chemical approach generalization for systems with weakly interacting electrons ultimately requires taking into account the electrons correlation and passing to computational schemes that involve full configurational interaction (CI). However, the traditional complete-active-space-self-consistent-field (CAS-SCF) methods that deal correctly with two electron systems of diradicals and some dinuclear magnetic complexes, cannot handle systems with a large number of the electrons due to a huge number of configurations generated in the active space of the system so that for m singly occupied orbitals on each of n identical centers $2mn$ Slater determinants should be formed by assigning spins up or down to each of the nm orbitals [1]. It has been accepted until recently, that CASSCF type approaches are non-feasible for many-odd electron systems such as fullerenes, CNTs, and graphene. Thus, addressing single-determinant approaches appeared to be the only alternative.

The open-shell unrestricted broken spin-symmetry (UBS) approach suggested by Noodleman [4] is well elaborated for both wave-function and electron-density QCh methodologies, based on unrestricted single-determinant Hartree-Fock scheme [5] (UBD HF) and the Kohn-Sham single Slater determinant procedure DFT (UBS DFT) [6]. The UBS approach main problem concerns spin-contamination of the calculation results. The interpretation of UBS results in view of their relevance to physical and chemical reality consists in mapping between the eigenvalues and eigenfunctions of exact and model spin Hamiltonians. While the implementation of UBS HF approach, both *ab initio* and semiempirical, is quite standard and the wished mapping is quite straightforward, this is not the case of the UBS DFT due to the problem with total spin. As known, DFT cannot be directly applied to calculation of the spin and space multiplet structure and a number of special procedures, that all are beyond the pure DFT scope [7], are suggested to overcome the difficulty. The procedures differ by computation schemes as well as by obtained results so that UBS DFT is theory-level-dependent [7, 8].

The paper presents a comparative analysis of the UBS HF and UBS DFT calculations results related to fullerenes, carbon nanotubes, and graphene. A comparison of the results to findings obtained with the application of many-body CI schemes [1, 2] highlights the UBS HF high ability to quantitatively describe practically important consequences of weak interaction between odd electrons of the studied nanocarbons.

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Contribution F.15 - Thursday, June 24

First-Principles Study of Physical Properties of Single ZnO Monolayer with Graphene-Like Structure

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The phonon dispersion relation, the elastic and piezoelectric constants, the specific heat at various temperatures, the electronic band structure, and the optical dielectric functions of a single ZnO monolayer (SZOML) with graphene-like structure are obtained from the first-principles calculations. The phonon dispersion curves contain three acoustic and three optical branches. At Γ point, the out-of-plane acoustic mode has an asymptotic behavior $\omega(q) = Bq^2$ with $B = 1.385 \times 10^{-7} \text{ m}^2/\text{s}$, while two in-plane acoustic modes have sound velocities 2.801 km/s and 8.095 km/s ; the other three optical modes have frequencies 250 cm^{-1} , 566 cm^{-1} , and 631 cm^{-1} . The elastic and piezoelectric constants reveal that the SZOML is softer than graphene, while it is a piezoelectric material. The specific heat increases with temperature. Its low-temperature behavior can be understood in terms of the phonon dispersion relation. The electronic band gap is 3.576 eV , which implies that the SZOML is a wide band gap semiconductor. Many peaks exist in the linear optical spectra, where the first peak at 3.58 eV corresponds to the band gap of SZOML.

Contribution F.16 - Thursday, June 24

Growth and characterization of single-walled carbon nanotube forests by remote plasma-assisted and thermal chemical vapor deposition

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Dense, vertically aligned single-walled carbon nanotubes (SWNTs) have been stimulating their application researches such as interconnects, thermal managements, supercapacitors, self-cleaning adhesive tapes, and chemical sensors. Their controlled growth, however, remains the main bottleneck towards their scalable integration, particularly when selective growth of SWNTs is required. Chemical vapor deposition (CVD) recipes for SWNT forests have been reported, typically focusing on process details, such as plasma enhancement, alcohol-based precursors and the effect of water addition.[1-5] Fundamental aspects, in particular the detailed role of reactive carbon and etching species created e.g. by a plasma or hot-filament during CVD, are difficult to extrapolate and hence are not well understood.

Here, we compare microwave plasma-assisted and thermal CVD in the same cold-wall reactor and for the same Fe/Al₂O₃ based catalyst substrates. Based on detailed mass spectroscopy for SWNT forest growth using remote microwave excitation of CH₄ diluted in H₂, we reproduce similar gas compositions for purely thermal CVD at nominally the same temperature. We thereby succeeded to grow dense, vertically aligned, mm-long SWNT forests by simple thermal CVD. This is not only relevant to process integration, but also allows us to elucidate the role of the plasma and key aspects of SWNT forest nucleation on a much more general level. We can exclude carbon precursor dissociation and the presence of highly activated gas species due to plasma excitation prior or during CVD as necessity of SWNT forest nucleation. Unlike previous reports on hot-wall CVD, we do not deliberately add any particular amount of water or oxygen to the growth atmosphere, and we also demonstrate the ability to selectively grow SWNTs on fully processed CMOS chips at room temperatures by using the on-chip built-in micro-hotplate as a local heater; therefore we find the results transferable to other cold-wall reactors.

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Contribution F.17 - Thursday, June 24

Intrinsic properties and complementary electronics of graphene nanoribbons

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Graphene nano-electronics has been very attractive due to high carrier mobility. The semi-metallic nature of bulk graphene requires width confinement down to ~sub-10nm in order to induce adequate bandgap for room temperature logic applications. We developed a unique chemical route to synthesize high quality, ultra-smooth graphene nanoribbons (GNRs) with width below 10nm. Transport measurements show that the bandgap scales inversely with GNR widths, indicating that bandgap opens in narrow GNRs due to quantum confinement. The first room temperature p-type graphene field-effect transistor (FET) is demonstrated with our chemically derived sub-10nm GNR.

We next access the performance of individual chemically derived sub-10nm GNR FETs. At on state, the current density could be as high as ~2000uA/um, with on/off ratio ~ 10⁶, subthreshold slope ~210mV/dec. The performance of sub-10nm GNR FETs is comparable to small diameter (d<1.2nm) carbon nanotube (CNT) FETs. The intrinsic carrier mobility and scattering mean free path is ~200cm²/Vs and ~10nm, respectively. We discuss the possible scattering mechanisms in the GNRs.

Compared to CNTs, GNRs have open edges with high chemical reactivity. We can take advantage of this fact and chemically modify the GNR edges to change the electronic properties. We found that individual GNRs could be covalently functionalized by nitrogen species through high-power electrical joule heating in NH₃ gas, leading to n-type electronic doping consistent with theory. The formation of C-N bond occurs mostly at the edges of graphene where chemical reactivity is high. X-ray photoemission spectroscopy and nanometer-scale secondary ion mass spectroscopy confirm the C-N species in graphene thermally annealed in NH₃. We fabricated an n-type N-doped graphene field-effect transistor (FET) that operates at room temperature.

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Contribution F.18 - Thursday, June 24

Tailoring the characteristics of graphite oxides by different oxidation times

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Graphite oxide was synthesized using various oxidation times and characterized by its physical and chemical properties. The degree of oxidation of the graphite oxide was systematically controlled via the oxidation time up to 24 hours. Three phases of interlayer distances were identified by X-ray diffraction: pristine

graphite (3.4 Å), intermediate (4 Å), and fully expanded graphite oxide (6 Å) phases. These phases were distinguished by an atomic ratio of O/C, which occurred from the different compositions of epoxide, carboxyl, and hydroxyl groups. The band gap of the graphite oxides was also tuned via the oxidation time, resulting in direct-band gap engineering from 1.7 to 2.4 eV, and strong correlation to the atomic ratio of O/C.

Contribution F.19 - Thursday, June 24

Hydrogen storage in ammonia borane: *Ab initio* study of the de- and rehydrogenation mechanisms

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Using *ab initio* density functional calculations, we study the microscopic mechanism of hydrogen release from ammonia borane (NH₃BH₃) and the reverse process leading to its subsequent recharging with hydrogen. Our total energy surfaces indicate the most favorable pathways to thermally convert the NH₃BH₃ molecular solid to the energetically preferred polymer NH₂BH₂ and molecular hydrogen. We found that energetically, tetragonal crystal structure can coexist with orthorhombic crystal structure around dehydrogenation temperature, and diammoniate of diborane (DADB) formation is helpful to make effective dehydrogenation in the crystal. To prevent formation of undesirable side-products such as the cyclic compound borazine (N₃B₃H₆) or other complexes that would prevent subsequent rehydrogenation, we propose to enclose AB in narrow carbon nanotubes. In this constrained space, we investigate possible rehydrogenation pathways using atomic and molecular hydrogen as well as selected protonation agents.

Contribution F.20 - Thursday, June 24

Carbon Nanotube Josephson Junctions with Nb Contacts

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We report on low temperature transport measurements on carbon nanotube Josephson junctions. We use a multiwall carbon nanotube (MWNT) as weak link and niobium as superconductor. To prevent premature switching of the junction we employ a low temperature filtering scheme and an on-chip resistive environment which provides damping at the plasma frequency of the junction. Depending on the applied gate voltage V_G we observe both, supercurrent and Coulomb blockade. The supercurrent versus V_G curves show a resonant behavior and, in average, the supercurrent increases when the gate voltage is tuned more negative. The IV characteristics are hysteretic and feature a small finite resistance in the superconducting branch that is typical for phase diffusion. We measure the temperature dependence of the critical current at one superconducting resonance and compare our results with a model for diffusive SNS junctions. In the Coulomb blockade region we focus on the magnetic field dependence of the linear conductance and find a splitting of Coulomb peaks.

Contribution F.21 - Thursday, June 24

Hybrid CMOS Device Utilizing Zinc Oxide Nanowire and Single Walled Carbon Nanotube Thin Film Transistors

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Zinc oxide (ZnO) nanowire and single walled carbon nanotube (SWCNT) networks have been proposed as an alternative to organic and amorphous semiconductors for plastic electronics. Although the mobility of the ZnO and SWCNT networks is lower than that of individual nanowires and nanotubes, they offer the advantages of high transparency and flexibility. A major drawback of using individual nanowires and nanotubes in nano or microelectronic applications is the lack of a manufacturable process to precisely assemble nanowires into small devices. The use of ZnO networks avoid this issue for relatively large area macroelectronic devices since the devices exhibit the average properties of a large number of random individual nanowires and nanotubes. In this work, we have deposited uniform ZnO nanowire and SWCNT thin films using an easy, scalable, stamping method and characterized their electronic properties. In addition, we have demonstrated a high performance and manufacturable hybrid complementary inverter (gain ~ 0.9) combining SWCNT networks as the p-type (hole carrier) thin film transistor (TFT) and ZnO nanowire networks as the n-type (electron carrier) TFT has been demonstrated for the first time.

Contribution F.22 - Thursday, June 24

Anisotropic spin-orbit splitting induced by curvature in carbon nanotubes

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Spin-orbit coupling in carbon nanotubes has been shown in recent experiments [1], rebutting the widespread idea of being negligible in carbon-based systems. Besides showing the importance of spin-orbit interaction in carbon nanotubes, Kuemmeth et al. [1] note an unexplained anisotropy in electron and hole levels.

In this work we study spin-orbit interaction in carbon nanotubes. We have found that, besides the dependence on diameter and chirality, spin-orbit effects are anisotropic: splitting is larger for the top valence band or bottom conduction band depending on the kind of nanotube [2]. Different tube behaviors are classified into three families, which are labeled with the so-called chiral index. Curvature changes the orbital hybridization in a family-dependent way. Our results are compatible with the reported electron-hole anisotropy without resorting to external fields, and predict a further dependence on the type of nanotube.

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Contribution F.23 - Thursday, June 24

Various Methods of Producing Suspended Graphene Nanoribbon Structures for their NEMS Applications

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In this presentation, we introduce a variety of methods to produce suspended graphene nanoribbon (GNR) structures. A single layer of graphene was exfoliated from graphite flakes on top of an SiO₂ substrate with pre-patterned coordinate markers. Suspended GNR structures were fabricated through three different methods: direct exfoliation on to a trench substrate, wet etching of the substrate, and the transfer-printing technique. The structures were investigated using micro Raman spectroscopy. The possible applications of these structures for Nanoelectromechanical Systems (NEMS) study will be discussed at the end of this presentation.

Zigzag Grows Faster Than Armchair: Comparisons of SWNT Growth From Self-Consistent-Charge Density-Functional Tight-Binding Molecular Dynamics Simulations

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The growth of single-walled carbon nanotubes (SWNTs) from Fe₃₈ clusters has been simulated using the self-consistent-charge density-functional tight-binding method, in conjunction with non-equilibrium molecular dynamics (SCC-DFTB/MD). Growth of the nanotube sidewall was induced by the supply of gas-phase atomic carbon at two different rates to randomly chosen sites in the Fe-C boundary region of both (5,5)-SWNT-Fe₃₈ and (8,0)-SWNT-Fe₃₈.^{1,2} Therefore, the dependence of SWNT growth dynamics on both the chiral angle of the SWNT (θ) and the rate of carbon supply were elucidated. SWNTs grown in this manner exhibited a large number of defects. In addition, SWNT healing was driven by the relative rates of defect removal and addition in the nanotube sidewall near the SWNT-Fe₃₈ boundary.³ The mechanisms by which 5-77-5, adatom and vacancy defects were removed from the SWNT generally took place over timescales of 1-10 ps. These mechanisms were therefore enhanced using lower rates of carbon supply. From comparison of the mean growth rates of (5,5)- and (8,0)-SWNTs, an inverse relationship between θ and the SWNT growth rate was established. In particular, (8,0)-SWNTs exhibited a mean growth rate *ca.* 10% greater than that of (5,5)-SWNTs during the early stages of growth. Recently reported data⁴ suggests that the converse is the case when SWNT growth is induced by the diffusion of carbon over the catalyst surface to the SWNT-catalyst boundary. It is concluded therefore that the energetic and kinetic properties of SWNT growth mechanisms, and therefore SWNT growth rates, depend on the manner in which carbon density is supplied to the nanotube itself (*i.e.* direct addition at the SWNT-catalyst interface, as opposed to addition following diffusion over the catalyst surface). It is also postulated that a dependence of SWNT growth rate on the form of carbon feedstock

supplied to the SWNT (*i.e.* C, as opposed to C_n) would be observed. The growth rates of (5,5)- and (8,0)-SWNTs observed in this work have been ascribed to the relative addition rates of 5-, 6- and 7-membered rings to the respective sidewall structures. In particular, carbon added to the (8,0)-SWNT-Fe₃₈ complex generally resulted in a more exclusive construction of 6-membered rings, and hence a faster, more linear extension of the (8,0) *sp*²-hybridized network, than observed for the (5,5)-SWNT case.

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Contribution F.25 - Thursday, June 24

Stability, chemical structure, and Clar's aromatic sextets of hydrogen-terminated graphene ribbons

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We determine the stability, the geometry, the electronic, and magnetic structure of hydrogen-terminated graphene-nanoribbon edges as a function of the hydrogen content of the environment by means of density functional theory [1]. Antiferromagnetic zigzag ribbons are stable only at extremely low ultrahigh vacuum pressures. Under more standard conditions, the most stable structures are the mono- and dihydrogenated armchair edges and a zigzag edge reconstruction with one di- and two monohydrogenated sites. At high hydrogen concentration “bulk” graphene is not stable and spontaneously breaks to form ribbons, in analogy to the spontaneous breaking of graphene into small-width nanoribbons observed experimentally in solution. The stability and the existence of exotic edge electronic states and/or magnetism is rationalized in terms of Clar's aromatic sextets.

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Contribution F.26 - Thursday, June 24

Thermal Transport in Controlled-Morphology Aligned-CNT Forests and Composites: Experimental and Numerical Comparative Studies

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The use of carbon nanotubes (CNTs) as a component of various materials, including polymer-based matrices for polymer nanocomposites (PNCs), to modify transport properties (electrical and thermal) has generated much research interest due to the wide variety of potential applications from aerospace to microelectronics. Thermal transport enhancement and tailoring has not been as successful as electrical conductivity enhancement, due to differences in electron and phonon transport and limiting mechanisms such as thermal barrier resistance. In this work, aligned multi-walled carbon nanotube (MWNT) forests embedded in a polymer are selected as a controlled and representative element to rigorously study such effects. Alignment of the CNTs along the heat conduction direction optimizes the effective thermal conductivity by minimizing the number of interfaces across the thermal path. Conduction perpendicular to the CNT axis will be studied as well and is dominated by thermal boundary resistance. Heat conduction in the CNT composites at room temperature are also simulated with parameters that describe behaviors at thermal interfaces. The experimental and numerical results are compared to quantify these parameter values for the first time. A significant advantage in our study is the capability to freely change the length and the spacing between the CNTs, and the type of polymer.

Vertically aligned MWNTs are grown through thermal chemical vapor deposition (CVD) to lengths of ~200-1000 um from an iron catalyst deposited on

silicon substrates. The MWNTs are delaminated from the substrate, and are uniaxially and biaxially densified to achieve various CNT volume fractions (~1-20%). In order to form CNT PNCs, densified forests are infiltrated and cured with a thermosetting polymer. The temperature gradient is measured along the CNTs by an infrared microscope, and is combined with a known heat flux to calculate the conductivity. Full-field thermal imaging allows and isolates the CNT-substrate thermal contact resistance from the CNT film thermal conductivity.

Thermal transport in CNT composite is numerically studied with a previously established off-lattice Monte Carlo simulation that uses a random walk algorithm, which is more efficient than molecular dynamics and finite element methods. Parameters are selected regarding essential CNT morphology, such as CNT orientation relative to heat transfer, CNT diameter, length, volume fraction, and thermal boundary resistances, and inter-CNT contact percentage. The simulated results are compared with the experimental data to evaluate the thermal boundary resistances.

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