Nanometer-scale Science and Technology Division
Room 6C - Session NS-MoM

Nanotechnology

Moderator: H.G. Craighead, Cornell University

9:00am **NS-MoM3 Nanotechnology - Fiction, Fad or Future?**, ***J.S. Murday,*** Naval Research Laboratory **INVITED**

Nearly 20 years have passed since Binnig and Rohrer published the first STM paper. This is the traditional gestation period for maturation of science into technology. What are the prospects for the science of nanostructures leading to new technology? There is already significant technology based on empirically derived nanostructures (for instance, heterogeneous catalysts, photographic film). A broad base of new nano-analytical tools is in place; nano-fabrication techniques are improving; new products are appearing in the market; and Federal funding agencies are taking notice. The National Science and Technology Council has formed an Interagency Working Group on Nanometer Science, Engineering and Technology. The working group will issue a report (June 1999) summarizing the opportunities, suggesting a national initiative in nanotechnology, and recommending a substantially larger federal investment in the science necessary to accelerate technologies built on nanostructures. This talk will briefly review the SOA in nanoscience, focus on highlighting examples where AVS pertinent nanoscience is making the transition into technology (computer memory-terabit/in2, biological sensors-molecular recognition/signal transduction, and nanostructured coatings-surface engineering), and conclude with a glimpse at potential federal agency funding.

9:40am **NS-MoM5 A Report on the Workshop "Vision for Nanotechnology R&D in the Next Decade"**, ***R.S. Williams,*** Hewlett-Packard Labs **INVITED**

More than 70 scientists, engineers, program directors and senior administrators from a broad array of disciplines, institutions and geographical regions gathered from January 27-29 in Washington, DC to discuss their views on the future of Nanotechnology research. This workshop was sponsored by the Interagency Working Group on Nano Science, Engineering and Technology (IWGN), which in turn has been charged by the Committee on Technology of the Office of Science and Technology Policy to identify the trends in nanotechnology, establish federal R&D priorities, and provide budget guidance to ensure that the potential of nanotechnology can be achieved in the US. Representatives from academic, corporate and government research organizations with backgrounds in dispersions and coatings, electronics broadly defined, composite structural materials, biology, medicine, energy and environmental sciences discussed technical issues and appropriate funding strategies. Given the large and heterogeneous nature of the workshop attendees, there were a surprising number of scientific themes that emerged as being crucial across the spectrum of research areas, such as ripening. If there were consensus issues among the attendees, they were most probably "Nanotechnology does not yet exist, but it will develop rapidly over the next decade", "avoid hype and extravagant promises", "the best federal investment strategy is to back a broad spectrum of high quality basic research and not focus on specific applications too soon", "focus the majority of funding on individual researchers and small interdisciplinary teams", and "the creation of nanotechnology will require the collaborative efforts of transdisciplinary teams and will in turn transform many traditional disciplines". This presentation will describe some of the accomplishments of current nanoscience research, opportunities for the future that were identified, and recommendations for funding agencies that came out of the workshop.

10:20am **NS-MoM7 Experimental and Theoretical Coincidence in Room Temperature Single Electron Transistor Formed by AFM Nano-Oxidation Process**, ***Y. Gotoh,*** *K. Matsumoto, T. Maeda,* Electrotechnical Laboratory MITI, Japan*; S. Manalis,* Massachusetts Institute of Technology*; J. Harris, C. Quate,* Stanford University

The experimental results of the room temperature operated single electron transistor (SET) were simulated using orthodox theory and 3 dimensional Poisson's equation. The simulated results coincided well with the experimental results. The planer type SET has been fabricated by oxidizing the surface of 2nm-thick titanium (Ti) metal that was on the atomically flat @ALFA@-Al@sub 2@O@sub 3@ substrate using the pulse mode AFM nano-oxidation process@super 1)@. The narrow oxidized Ti wire works as a tunnel junction for SET. The fabricated SET shows Coulmb oscillation characteristic even at room temperature at the drain bias of V@sub D@=0.3V when the gate bias was changed from V@sub G@=0 to 10V, and 5 oscillation peaks were observed with the periods of ~2V. The drain current was modulated by the gate bias and oscillates from 2.4pA to 3pA. Therefore, the modulation rate is ~20%. Using the orthodox theory, the experimental Coulmb oscillation was fitted using the parameters of the gate capacitance CG=8x10@super-20@F and the tunnel junction capacitances C@sub 1@=C@sub 2@=2.9x10@super -19@F. The simulated result represents well the experimental one, i.e. the position and the number of the Coulmb oscillation peaks and the modulation rate of the drain current coincide with the experiment of ones. Furthermore, tunnel junction capacitances were calculated by solving the 3D Poisson's equation for the structures of fabricated SET. In the calculation, the error tolerance of 0.01% was used. The calculated tunnel junction capacitances is found to be C@sub 1@=C@sub 2@=4x10@super-19@F which is almost coincide with the parameter used in the orthodox simulation. For further improvement of SET characteristics, an ultra sharp multi-wall carbon nanotube AFM tip was introduced for the AFM nano-oxidation process to reduce the oxide wire width down to 10~15nm to increase a tunnel current to improve S/N ratio of SET. 1) K. Matsumoto, Proceedings of IEEE Vol. 85, No. 4, p. 612 (1997).

10:40am **NS-MoM8 Study of the Super-resolution Near-field Structure for Optical Storage**, ***F.H. Ho,*** *D.P. Tsai, C.W. Yang,* National Chung Cheng University, Taiwan

We present the study of the mechanism of surface plasmons enhanced super resolution near-field structure, glass/SiN/Sb/SiN, for optical storage. Nonlinear near-field optical effects of the glass/SiN/Sb/SiN on the transmitted light spot were experimentally observed by a tapping-mode tuning fork near-field scanning optical microscope. Imaging results of the near-field intensity gradients showed that focused light spot through the super resolution optical near-field structure, glass/SiN/Sb/SiN, consists of a normal propagating term and an evanescent term resulting from the laser-excited surface plasmon of the Sb thin film. Results also demonstrated the spot size of the evanescent field intensity can be manipulated by the detecting sensitivity of PMT, while the spot sizes of the propagating intensity remained the same. The working principle of the reduction of the focused spot size and the transfer of near-field photo-thermal energy from Sb/SiN interface to the recording layer are explained.

11:00am **NS-MoM9 Nanometer-scale Science of Conjugated Polymer Interfaces**, ***A.R. Burns,*** *R.W. Carpick, D.Y. Sasaki,* Sandia National Laboratories

Highly-ordered organic films with integrated conjugated backbones and functionalized tail groups have considerable promise in several areas of nanometer-scale science and technology, especially sensor development. This technology brings together synthetic strategies, self-assembly and Langmuir-Blodgett deposition, and scanning probe characterization of both structural and optical responsivities. Specifically, we will discuss recent developments in the preparation and analysis of polydiacetylene monolayers on silica and mica substrates. As confirmed by atomic force microscopy and fluorescence microscopy, the monolayers consist of domains of linearly oriented conjugated backbones with pendant hydrocarbon side chains above and below the backbones. The backbones impose anisotropic packing of the hydrocarbon side chains which leads to a 300% friction force anisotropy. Phase transitions of the polymer induced by localized mechanical strain or chemical binding will also be discussed in terms of optical and morphological changes. Finally, we will discuss results concerning the incorporation of these polymers into three-dimensional nanocomposites. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

11:20am **NS-MoM10 Fabrication of Nanostructures by Laser Focusing of Fe Atoms**, ***R.C.M. Bosch,*** *K. van Leeuwen, H.C.W. Beijerinck,* Eindhoven University of Technology, The Netherlands

We present an improved atom lithography method for the production of nanomagnetic wires and dots having well defined shape and separation. It is based on laser manipulated deposition of a supersonic beam of Fe atoms. The nodes of a 372 nm standing light wave act as a perfect lens for an incoming monochromatic parallel atomic Fe beam. The feature size of the deposited structures is therefore first of all limited by the quality of the incoming beam, and secondly by spherical aberration. A parallel beam is obtained by well known laser cooling techniques, but our improvement lies in the reduction of chromatic aberration by using a self-developed Fe evaporation source seeded with high pressure argon gas. The mixture will

expand supersonically and due to adiabatic cooling it is in principle possible to obtain a beam with an axial velocity spread of less than 10%. The problem of spherical aberration will be solved with beam masking: a transmission grating with 100 nm slit sizes upstream of the standing wave allows only atoms near the nodes to be deposited. With the presented method we expect to reduce the structure sizes produced by conventional atom lithography methods and to break the 10 nm limit.

11:40am **NS-MoM11 One-dimensional Nanostructure of SiCN Single Crystal**, ***P.F. Kuo***, National Taiwan University, Taiwan; *C.-Y. Wen,* National Taiwan University; *F.G. Tarntair,* National Chio Tung University, Taiwan; *J.-J Wu,* Institute of Atomic and Molecular Sciences, Taiwan; *S.L. Wei,* Fu-Jen University, Taiwan; *K.H. Chen,* Academia Sinica, Taiwan; *L.C. Chen, Y.F. Chen,* National Taiwan University

Nanostructural materials have attracted wide attention due to its fundamental confinement effect and further applications of composites and microelectronics. From the standpoint of one-dimensional structures, there has been significant speculation about structures and properties of nanotubes and nanorods. In this paper, we report the growth of a novel one-dimensional single crystal nanorod comprised of Si, C, and N using microwave plasma enhanced chemical vapor deposition (MWCVD). The transmission electron microscopic analysis shows that the nanorods are of 1.5 μm in length and 50 nm in diameter, and the lattice images indicate that they are single crystals. High-resolution scanning electron microscope further confirms the nanorod diameter ranging from 10 to 60 nm, with hexagonal cross-section. The stoichiometry of the crystal was examined by the energy dispersive X-ray spectrometer (EDX) and the results showed a Si, C, N atomic ratio of 1:2:1. Detailed structural and stoichiometry information as well as optical and electronic properties measured by photoluminescence (PL) and electron field emission measurement are reported in this paper.

Nanometer-scale Science and Technology Division
Room 612 - Session NS1-MoA

Nanoscale Tribology and Adhesion

Moderator: S.S. Perry, University of Houston

2:00pm **NS1-MoA1 Tribological Properties of Self-Assembled Monolayers on Si Surfaces**, ***J.E. Houston***, *J.D. Kiely,* Sandia National Laboratories; *J.A. Mulder, X.-Y. Zhu,* University of Minnesota

The use of organic monolayers as lubricating films has recently received considerable attention, especially with regard to their potential use in micromachine applications. We have used the interfacial force microscope (IFM) to characterize, on the nanometer scale, the tribological properties of a new class of self-assembled monolayers on Si(001) surfaces. These films consist of alkyl-OH and NH2 terminated molecules reacted with a fully chlorinated Si surface. We contrast their tribological behavior with those of the more familiar alkylchlorosilane monolayers through measurements of contact hysteresis, lateral frictional force and film conductance as a function of normal load. In addition, we probe the wear behavior under repetitive "wear-track" cycles. The chlorosilane monolayers show high friction coefficients and considerable wear while the films grown on the chlorinated surface show low friction coefficients and little wear, suggesting that the latter has considerable potential as a monolayer lubricant for Si. We discuss these results in terms of what is known concerning the structural and chemical properties of these two types of self-assembled monolayers. This work was supported by the U.S. Department of Energy under contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U.S. Department of Energy.

2:20pm **NS1-MoA2 Contact Hysteresis, Friction and Conductance of Self-Assembled Monolayers on Au**, ***J.D. Kiely***, *J.E. Houston,* Sandia National Laboratories

We have investigated the relationship between friction and the mechanical, electrical and chemical properties of self-assembled monolayers of hexadecanethiol on the Au(111) surface using the interfacial force microscope. We find a very low friction coefficient for freshly prepared films with a direct correlation of the frictional force with the contact hysteresis, i.e., the energy dissipated in the film during a loading/unloading cycle. In addition, the film conductance is found to increase exponentially with the applied film stress under loading. Above film stresses of about 4 Gpa, the film compliance and frictional force rise sharply while the conductance remains log linear. To simulate aging in a laboratory environment, we have oxidized films by direct exposure to ozone and find that the frictional force, conductance and hysteresis all rise dramatically. We discuss these results in terms of the known properties of the monolayer films and the findings of previous work on the effects of oxidation by ozone exposure. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

2:40pm **NS1-MoA3 Energy Dissipation in Defective Alkanethiol Monolayers**, ***N.D. Shinn***, *J.D. Kiely, J.E. Houston,* Sandia National Laboratories

Although highly ordered, alkanethiol self assembled monolayers (SAMs) have a hierarchy of structural defects that lead to dynamic energy dissipation.@footnote 1@ Counter-intuitive friction results on nominally isomorphic monolayers suggest surprising sensitivity to subtle structural differences or demonstrate that extrinsic probe/monolayer interactions dominate friction.@footnote 2@ We separate intrinsic and extrinsic contributions to friction by using a Quartz Crystal Microbalance to inertially shear and simultaneously measure the intrinsic energy dissipation in pure, mixed and damaged alkanethiol SAMs chemisorbed on Au(111)-textured QCM electrodes. For complete monolayers, domain boundaries are the major symmetry-breaking defects that enable dissipation. Point defects created by electron or UV irradiation only incrementally increase the intrinsic dissipation. Residual fluid phases, most notably in sub-monolayer films, lead to the highest dissipative losses. Oxidation by ozone decouples the SAM from the Au(111) substrate and dramatically increases the intrinsic dissipation. Interfacial Force Microscope experiments demonstrate how the structure-dependent SAM viscoelasticity is manifested in controlled friction measurements.@footnote 3@ Research supported by DOE-BES Materials Sciences. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000. @FootnoteText@@footnote 1@N. D. Shinn, T. M. Mayer and T. A. Michalske, Tribology Letts. (in press). @footnote 2@ H. I. Kim, T. Koini, T. R. Lee and S. S. Perry, Langmuir 13, 7192 (1997). @footnote 3@J. E. Kiely, N. D. Shinn and J. E. Houston, Langmuir (submitted).

3:00pm **NS1-MoA4 Interaction Forces Measured with Functionalized Cantilevers and SFM Modulation Techniques**, ***A.L. Szuchmacher***, *R. Luginbuehl, T. Engel, R.M. Overney,* University of Washington

Understanding local interaction forces between material surfaces is very important for many industrial and research applications such as tribology, materials science, bioengineering, and polymer science. The scanning force microscope allows for measuring forces acting at those interfaces. In order to understand the interactions between probe and material surfaces, the surface chemistry of the SFM tip must be well defined. Ultrasharp silicon cantilevers were reacted with different silanes to produce well defined and covalently bound monolayer films. The quality of these coatings was controlled by different techniques including ESCA and SFM. These tips were used to study the interactions of thin films using force-displacement curves and friction force measurements. Special SFM modulation techniques were applied to probe and image the interfacial interactions. Amplitude and phase response signals will be discussed. Fundamental effects of solvents on van der Waals interactions between surfaces were investigated as well as hydrogen bonding effects. Experiments were carried out as a function of surface chemistry, temperature, solvent, and pH.

3:20pm **NS1-MoA5 SPM Tip-Sample Interactions in Primary Alcohols of Varying Chain Length**, ***R.M. Ralich***, *Y. Wu, R.D. Ramsier, P.N. Henriksen,* University of Akron

Interactions between functionalized tips and substrates in scanning probe microscopy (SPM) are usually investigated by utilizing an intervening liquid medium, however the results may be influenced in various ways by the medium itself. In this study the chain length of a series of primary alcohols is shown to affect adhesion measurements. The measurements are performed between a layer of phosphonic acid adsorbed on an aluminum substrate and an aluminum-coated, hydroxyl-terminated silicon nitride tip. These are adsorption systems that have been characterized previously by vibrational spectroscopy and form a stable, well-defined system for studying the effects of the medium on adhesion. Adhesion forces between the tip and sample are observed to decrease as the alcohol chain length is increased. These data imply that a synergistic combination of fundamental interactions is responsible for adhesion in this system.

3:40pm **NS1-MoA6 Sliding Friction of Xenon Monolayers and Bilayers on Pb and Cu Substrates**, ***S.M. Winder***, *B. Mason, J. Krim,* North Carolina State University

Studies of the fundamental origins of friction have undergone rapid progress in recent years with the development of new experimental and computational techniques for measuring and simulating friction at atomic length and time scales.@footnote 1@ The increased interest has sparked a variety of discussions and debates concerning the nature of the atomic-scale mechanisms that dominate the dissipative process by which mechanical energy is transformed into heat. We report here our measurements of the sliding friction of xenon monolayers and bilayers sliding on Cu and Pb surfaces. Such studies provide information on the relative contributions of electronic and phononic dissipative contributions to sliding friction, since phonon dissipation is present at all film coverages, while electronic dissipation primarily impacts the monolayer. For the system Xe/Pb the relative contributions of monolayer and bilayer coverages to the measured friction appear similar to those of Xe/Ag(111).@footnote 2@ This indicates the primary mechanism of friction in Xe/Pb and Xe/Ag is through phonons within the adsorbate. The substrate Pb is of particular interest on account of the recent observation of superconductivity-dependent sliding friction on this metal. The system Xe/Cu is interesting because the interaction potential of Xe/Cu is known accurately, allowing highly reliable comparisons of theory to experiment. Work funded by NSF DMR#9896280. @FootnoteText@ @footnote 1@ J. Krim, Scientific American, vol. 275, pp 74-80 (1996). @footnote 2@ C. Daly and J. Krim, Physical Review Letters, vol. 76, pp 803-806 (1996).

4:00pm **NS1-MoA7 Tribological Proprties of Single Crystalline Metal Surface**, ***A.J. Gellman***, *J.S. Ko,* Carnegie Mellon University **INVITED**

The tribological properties of single crystal metal surfaces have been measured under the ultra-high vacuum conditions of a surface analysis apparatus. This experiment allows us to measure both friction and adhesion between two single crystal surfaces brought into contact under a

wide range of loads, and sheared with a wide range of sliding velocities. Most importantly it is possible to maintain strict control over the chemistry and properties of the surfaces. The experiments performed to date have systematically varied a number of surface characteristics in order to observed their effects on tribological properties. The clean surfaces of singles crystals can be brought together under varying orientation. Experiments with Ni(100) surfaces have shown that the crystallographic orientation can affect the frictional properties of the interface. These result in variations of the friction coefficients over a fivefold range. Furthermore the effects of crystallographic oreintation propagate through adsorbed layer of thickness up to four monolayers. The effects of orientation are thought to result from plastic deformation in the bulk solid of the metal crystals. The effects of adsorbed species can be measured with an extremely high level of control over the nature of the adsorbate, its coverage and its chemistry. On both Cu(111) and Ni(100) surfaces we have observed that at coverages less than one monolayer adsorbed species have little or no influence on interfacial friction. This has been observed using both atomic and molecular adorbates. It is thought that for adsorbed films at coverages less than one monolayer direct metal-metal junctions across the interface cause displacement of adsorbed species from the contact region. The result is a metal-metal interface with high shear strength similar to that formed between clean surfaces. Finally, the friction between single crystal surfaces can be influenced by fine characteristics of the structure of adsorbed layers. Measurements reveal discontinuous breaks in the friction versus adsorbate coverage for both trifluoroethanol on the Cu(111) surface and ethanol on the Ni(100) surface. These discontinuities are attributed to layering of the adsorbate on the surface. The observation of such effects has been made in several laboratories using the surface forces apparatus to measure friction between perfectly flat mica surfaces. It is remarkable to see similar effects occuring between crystalline metallic surfaces that are plastically deformable.

4:40pm **NS1-MoA9 Combined Quartz Crystal Microbalance and Scanning Probe Microscope Studies of Vapor-Deposited Films on Metal Surfaces***, **B. Borovsky**, M. Abdelmaksoud, J. Krim,* North Carolina State University

Experimental investigations of friction, lubrication and adhesion at nanometer lengthscales have traditionally been performed by employing force microscopy, surface forces apparatus (SFA), or quartz crystal microbalance (QCM) techniques. While collectively these techniques have yielded much useful information, their results have to date never been mutually cross-referenced. In order to achieve such a cross referencing, we have performed two sets of measurements: (1) A QCM study of the system toluene/Ag(111) with and without C@sub 60@ vapor-deposited on the Ag(111) surface, and (2) a joint QCM/SPM study of the systems Ethylene/Pt and Oxygen/Ag. The former system has been studied by means of SFA,@footnote 1@ whereby it was reported that C@sub 60@ at a toluene/mica surface resulted in a significant reduction in friction levels. The latter studies allow direct comparison of SPM and QCM data, as the measurements are carried out in unison. Our studies of toluene/C@sub 60@ have revealed that the decrease in friction reported in Ref. 1 is most likely due to the manner in which the C@sub 60@ layer adheres to the solid substrate. Meanwhile, we have observed that for ethylene and oxygen adsorbed on Ag, a measurable shift in the frequency and amplitude response of the QCM occurs as the STM tip is dragged through the adsorbed layers. Additionally, allowing rubbing to proceed for extended periods within a small scanned region produces a large contrast with the surrounding region in STM images. The experiment is currently being repeated on a Pt substrate in order to search for a tribochemically-triggered reaction. Work funded by AFOSR F49620-98-1-02-1 and NSF DMR9896280 @FootnoteText@ @footnote 1@ S.E. Campbell, G. Luengo, V.I. Srdanov, F. Wudl and J.I. Israelachvili, Nature, volume 82, p 520 (1996) .

5:00pm **NS1-MoA10 Sliding Transitions and Dissipation in Nanoscale Contacts***, **K.J. Wahl**,* Naval Research Laboratory*; S.A.S. Asif,* University of Florida

In order to investigate tribological processes at the nanometer scale, we need to better understand how model asperity contacts respond to shear and dissipate energy. In our experiments, we investigate the dynamic processes occurring during the transition from static to sliding contact, as well as during the formation and breaking of nanoscale adhesive contacts. Measurements are made using an atomic force microscope operated in shear modulation mode, where the sample position is modulated laterally with amplitudes as small as a few Å. Both amplitude and phase response of the contacts are monitored using a lock-in amplifier. In this work, we expand our technique to incorporate harmonic analysis of the response of the contact to lateral modulation. As a result, we are now able to distinguish between various types of dissipation including friction, microslip and damping. We demonstrate application of this technique to discriminate between static to sliding contacts as well as identify and quantify microslip in nanoscale contacts.

Nanometer-scale Science and Technology Division
Room 6C - Session NS2-MoA

Quantum Dots and Wires

Moderator: M. Weimer, Texas A&M University

2:00pm **NS2-MoA1 High Resolution Optical Spectroscopy and Control of Single GaAs Quantum Dots***, **D. Gammon**,* Naval Research Laboratory **INVITED**

Recently it has become possible to probe individual excitons localized laterally in narrow GaAs quantum wells using high spatial and spectral resolution optical techniques. Discrete, atomic-like spectra with homogeneously-broadened linewidths as narrow as a few tens of micro-eV have been measured. These linewidths are two orders of magnitude narrower than the ensemble linewidth arising from inhomogeneous broadening and an order of magnitude narrower than the narrowest observed in wide quantum well samples. This extraordinary reduction in linewidth can be explained in part by the removal of inhomogeneous broadening accomplished by probing individual localized excitons, and in part by the reduction in homogeneous linewidth in going from 2D to 0D. In fact, the linewidths are in the regime expected for the intrinsic broadening mechanisms of exciton-phonon interactions and radiative emission. In other words the linewidths may be close to their natural linewidths.@footnote 1@ This great reduction in linewidth attained in PL by probing individual QDs has led to a number of new observations including fine structure splittings,@footnote 2@ hyperfine structure splittings @footnote 3@ and the measurement of the nonlinear response of a single quantum dot.@footnote 4@ Using coherent picosecond pulses, coherent control and the generation of superposition states have been demonstrated.@footnote 5@ These examples of advanced spectroscopies on individual excitons are first steps toward what may eventually lead in its maturity to coherent optical control of QDs comparable to what is now possible in atoms. @FootnoteText@ @footnote 1@ D. Gammon, et al., Science 273, 87 (1996). @footnote 2@ D. Gammon, et al., Phys. Rev. Lett. 76, 3005 (1996). @footnote 3@ S.W. Brown, et al., Phys. Rev. B 54, R17339 (1996); D. Gammon, et al., Science 277, 85 (1997). @footnote 4@ N. H. Bonadeo, et al., Phys. Rev. Lett. 81, 2759 (1998). @footnote 5@ N. H. Bonadeo, et al., Science 282, 1473 (1998).

2:40pm **NS2-MoA3 Quantum Dots; The Small World of Artificial Atoms***, **L.P. Kouwenhoven**,* Technical University of Delft, The Netherlands **INVITED**

We performed transport experiments on quantum dots in which the electron number can be tuned from 0 to 1, 2, etc. The addition spectrum shows a shell structure corresponding to a 2D harmonic confinement potential. The magnetic field dependence shows that the single particle states are spin degenerate and filled with two electrons. The filling of a shell occurs according to Hund's rule: electrons occupying degenerate states prefer to have parallel spins which lowers the total energy due to an increased exchange interaction. We observe such Hund's rule states at zero magnetic field and also at level crossings in a finite magnetic fields. In non-linear transport characteristics also the first few excited states are visible which we have studied over a magnetic field range up to 16 Tesla. The magnetic field induces transitions between ground states and excited states and also between excited states. In the high magnetic field regime all electrons are in the lowest orbital Landau level. This is the quantum Hall regime for a small electron system where the electrons form a strongly interacting many-body system. We have observed in the few-electron regime (N<10) so-called singlet-triplet oscillations. On increasing the magnetic field for a fixed electron number, we first observe spin-flips (between the two spin states of the lowest orbital Landau level), then the maximum density droplet (when all electrons are spin polarized and occupy the state with the lowest angular momentum), and then a reconstruction (probably an edge reconstruction, either spin polarized or with a spin texture). @FootnoteText@Work done in collaboration with D. Austing, M. Eto, T. Honda, S. Tarucha, M. Danoesastro, J. Janssen, R. van der Hage, and T. Oosterkamp.

3:20pm **NS2-MoA5 Low-Temperature Tunneling Spectroscopy of the Tip-induced Quantum Dot on n-InAs(110)**, *R. Wiesendanger,* ***M. Morgenstern****, R. Dombrowski, Ch. Whittneven,* University of Hamburg, Germany

The local tip-induced band bending in scanning tunneling microscopy (STM) studies of semiconductor surfaces leads to a quantum-dot-like potential. Scanning tunneling spectroscopy (STS) on n-InAs(110) at negative sample bias has been applied to determine the energies of the quantized states of the tip-induced quantum dot. Additionally, the magnetic-field dispersion of these states has been studied showing clearly the expected splitting of the first excited state in agreement with Hartree-Fock calculations. At positive sample bias the local tunneling spectra were found to be dominated by the Landau bands of the tip-induced quantum dot. Moreover, spatially-dependent spin splittings of the Landau bands were observed, induced by the spatially varying spin polarization of the tip-induced quantum dot.

3:40pm **NS2-MoA6 Coherently Strained Sn Quantum Dot Formation in Si via Phase Separation**, ***K.S. Min****, H.A. Atwater, N.J. Choly,* California Institute of Technology

Diamond cubic @alpha@-Sn is a zero band gap semiconductor and band structure calculations predict a direct and tunable energy gap for Sn-rich Sn@sub x@Si@sub 1-x@ alloy system. One approach for realization of a direct band gap material based on coherently strained Sn-rich Sn@sub x@Si@sub 1-x@/Si system is to synthesize coherently strained Sn-rich quantum dots. For high Sn concentration Sn@sub x@Si@sub 1-x@/Si quantum dot structures, one might potentially take advantage of quantum carrier confinement to further tune the energy gap over a wide range in the infrared frequency range. The biggest difficulty in growing Sn@sub x@Si@sub 1-x@ quantum dots via conventional epitaxial growth techniques, however, is the strong tendency for Sn atoms to segregate to the surface during growth at ordinary Si epitaxy temperatures. We report a novel two-step process for synthesizing coherent Sn-rich quantum dots contained within Si, where the enthalpy of mixing is highly positive. First, an ultrathin homogeneous Sn@sub x@Si@sub 1-x@ metastable solid solution sandwiched between Si is grown by temperature-modulated molecular beam epitaxy. The as-grown epitaxially stabilized ultrathin homogeneous film is then thermally annealed in high vacuum, whereupon the quantum dots precipitate as the ultrathin alloy film phase separates. The quantum dots appear in planar-view transmission electron micrographs as square-shaped with facets along the elastically soft direction. The mean size ranges from 2 nm to 3 nm for annealing temperature between 500°C and 800°C. Cross-sectional high-resolution transmission electron microscopy reveals that the dots are completely coherent with the Si matrix. The early stage of phase separation proceeds via spinodal decomposition, followed by diffusion-limited coarsening in the late stage. The optical properties of the quantum dots will also be presented.

4:00pm **NS2-MoA7 Hybrid Electrochemical/Chemical Routes to Epitaxial, Luminescent, and Size Monodisperse Semiconductor Nanocrystals on Surfaces.**, ***R.M. Penner****,* University of California, Irvine

A fundamentally new approach for synthesizing semiconductor nanocrystals - size-selectively - is described in this talk. Cadmium sulfide (CdS) nanocrystallites (NCs) have been synthesized on the atomically smooth graphite basal plane surface using a hybrid electrochemical/chemical (henceforth E/C) method. This method involves the following steps: 1) Electrochemical deposition of cadmium NCs onto an electrode surface, 2) Electrochemical oxidation of cadmium NCs to yield cadmium hydroxide (hexagonal) Cd(OH)@sub 2@ and, 3) Displacement of oxygen (or hydroxide) by sulfide either in the gas phase (via H@sub 2@S at 300 K) or in the liquid phase (using aq. Na@sub 2@S) solution. Electron diffraction is employed to monitor the progress of this synthesis, and the c rystal structures and orientations of the resulting nanocrystals which have mean diameters ranging from 30Å to 150Å. Wurtzite phase CdS nanocrystals generated by the E/C method possess the following characteristics: Single crystallinity, good-to-excellent si ze monod ispersity, epitaxial alignment (with the hexagonal periodicity of the graphite(0001) surface). In addition, E/C deposited particles on graphite exhibit strong room-tempera t ure photoluminescence (PL) spectra in which virtually no trap state emis sion is o bserved, and the energy of the emitted phonons is tunable based on the crystallite diameter. Extraordinarily good size monodispersity is possible for the CdS nanocrystals prepared by this method. One consequence is that the PL emission line widths seen for ensembles of 300,000 CdS nanocrystals can be as narrow as those seen for single CdS nanocrystals (15 meV at 20 K). V.

4:20pm **NS2-MoA8 High-Bias Conductance of Au Nanowires at 4 K**, ***A. Sakai****, K. Yuki,* Kyoto University, Japan

We have studied the bias dependence of the quantized conductance of Au nanowires at 4 K. The experiment was carried out on Au relay contacts which were directly immersed in liquid He. A well-defined 1G@sub 0@ peak (G@sub 0@=2e@super 2@/h is the conductance quantum unit) appears in the conductance histogram, as observed in previous work.@footnote 1@ With increasing the bias, the 1G@sub 0@ peak decreases in height, while its position remains unshifted. This behavior of the 1G@sub 0@ peak is just the same as that observed at room temperature.@footnote 2@ The critical bias V@sub c@ at which the 1G@sub 0@ peak disappears is 2.4 V, which is slightly higher than the values at room temperature (1.9 V) and at 77 K (2.2 V). This weak temperature dependence of V@sub c@ implies that the high-bias instability of the 1G@sub 0@ state of Au is not due to Joule heating effects. Our experimental results are rather consistent with the electromigration of contact atoms which predicts linear and moderate increase in V@sub c@ with decreasing temperature. @FootnoteText@ @footnote 1@J. L. Costa-Krämer, N. García, and H. Olin, Phys. Rev. B 55, 19 (1997). @footnote 2@H. Yasuda and A. Sakai, Phys. Rev. B 56, 1069 (1997).

4:40pm **NS2-MoA9 Quantized Conductance of Metal Nanowires: Is It Useful as a New Device?**, ***K. Takayanagi****,* Tokyo Institute of Technology, Japan **INVITED**

As the scale of microelectronic engineering continues to shrink, interest has focused on the quantum nature of electron transport through quantum wires and/or carbon nanotubes and electron storage on quantum dots. We report here firstly measurements of the quantized conductance of metal quantum poin contacts (QPC's) prepared with an STM that we can simultanelusly image using ultra-high vacuum (UHV) electron microscope. This STM-UHV electorn microscope technique allows us to directly observe any relationship between the structure and conductance of the QPC's. We observed gold metal QPC's, and found a single chain of gold atoms suspended between the electrodes. We can thus confirmed that the conductance of a single strand of atoms is 2e@super 2@/h, (13k@ohm@)@super -1@ , where 'e' is the electron charge and 'h' is Planck's constant. The QPC's often can form a very long nanowire suspended between the electrodes, which are ideal one-dimensional channel similarly to carbon nanotubes. To verify structures of such long matal wires, we made stable nanowires by electorn beam irradiation onto a very thin gold film. We first obtained high-resolution images of a linear chain which consists of four suspended gold atoms. The gold atoms had anomalous spacing compared with the nearest neighbor distance of the bulk crystal. Second, the nanowire which appears as three or four atom rows the diameter in TEM images have a structure different from the bulk crystal. It is very promising for microelectronic engineering that long gold nanowires have thier own specific structure and, thus, have definit conductances specific to their structures. @FootnoteText@ H.Ohnish, Y.Kondo, and K.Takayanagi, Nature, 395 (1998) 780.

Nanometer-scale Science and Technology Division
Room 612 - Session NS1-TuM

Nanomechanics

Moderator: B. Unertl, University of Maine

8:20am **NS1-TuM1 A Progress Report on the Road to Quantitative Nanotribology**, ***R.W. Carpick***, Sandia National Laboratories **INVITED**

The goal of routinely acquiring reliable, quantitative nanomechanical and nanotribological measurements with scanning force microscopy (SFM) has not yet been reached. As we travel along the exciting road toward this goal, several signposts warning us of the complications and drawbacks of SFM techniques have been recorded. In this talk I will discuss the current state of affairs regarding accurate measurement of mechanical and tribological properties at the nanometer scale. The critical roles of force calibration, tip characterization, cantilever properties and accurate displacement control will be discussed. Particular attention will be paid to the case of normal and lateral force measurements with contact-mode SFM. I will investigate the application of continuum mechanics models to SFM measurements, including recent models relating fracture mechanics and sliding friction measurements. Finally, I will discuss advantages gained by using novel instrumental approaches. * Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

9:00am **NS1-TuM3 Contact Properties of Oxide Surfaces: Long Range Forces and Adhesion**, ***E. Barthel***, *A.S. Huguet, R. Roquigny, S. Sounilhac,* CNRS / Saint Gobain Recherche, France **INVITED**

Surface Forces Microscopy (SFM) is useful to caracterize adhesive properties of surfaces. In practice, however, the usual relations between pull-off force and adhesion energy (JKR, DMT) may sometimes be inadequate, because the assumptions inherent to these models are not fulfilled. Using a general approach to the adhesive contact problem, based on Sneddon's results, and specific descriptions of the interaction(s) relevant to the cases under study, we will consider three non-trivial cases: 1) Silica/silica contact: in this case, both very short-range and long-range interactions contribute. We show how to split the total adhesion energy into its long-range and short-range contributions.@footnote 1@ 2) Surfactant monolayers: recent experiments@footnote 2@ have evidenced a power law dependance of the pull-off force as a function of driving velocity when surfactant monolayers are deposited on the surfaces. We provide an analytical model for this case, where viscoelastic losses are essential 3) Metal/oxide contact: using an UHV AFM, we have investigated the tungsten/oxide adhesion and long range forces.@footnote 3@ Short-range forces are shown to form the main contribution, although we did not achieve quantitative assesment. CONCLUSION Surface Forces measurements are a versatile tool for understanding interaction and adhesion properties of oxide surfaces. However, the bare pull-off force may reflect a variety of phenomena, which have to be properly taken into account in the data treatment. @FootnoteText@ @footnote 1@ Barthel E., Colloids and Surfaces A, 1999, 149, 99. @footnote 2@ Ruth M. and Granick S., Langmuir, 1998, 14, 1804. @footnote 3@ Sounilhac S., Barthel E. and Creuzet F., J. Appl. Phys., 1999, 85, 222.

9:40am **NS1-TuM5 Metallic Adhesion and Tunneling at the Atomic Scale**, ***A. Schirmeisen***, *G. Cross, A. Stalder, P. Grutter,* McGill University, Canada; *U. Durig,* IBM Research Division, Zurich Research Laboratory

We have measured forces and currents between atomically defined W(111) tips and a Au(111) sample in ultra high vacuum at 150 K. The W tips are manipulated and characterized on an atomic scale both before and after the experiment by field ion microscopy (FIM). The force-distance curve shows a peak of the attractive, adhesive metallic force of 5 nN for a three atom tip. Unexpected for a metallic system, there is no spontaneous jump-to-contact (Cross et al., PRL 80. 4685 (1998)). An analysis of the tip by FIM after the approach reveals an atomically unchanged tip apex even for repulsive forces of up to several nN. From a fit of our data to the Maugis-Dugdale theory we can determine that our system is close to the rigid body Bradley limit. The experimental data is described very well with a scaled Rydberg function with an unexpected large decay length of 0.2 nm. The simultaneously measured tunneling current has the expected exponential dependence on tip-sample separation, giving a reasonable barrier height of 3.7 eV. After a model proposed by Chen (J. Phys. Cond. Mat 3, 1227 (1991)) there should be a direct correlation between the tunneling current and adhesion force. Using our experimental data we extract a value for the LDOS of the W trimer tip of 1 state/eV/atom at the Fermi energy, which is in agreement with theoretical predictions. Finally, we have measured the evolution of the tip-sample contact for a tip radius of 3 nm and repulsive loadings as large as 200 nN. Half of these measurements show little or no hysteresis, whereas in the remaining indications of reversible slip behavior was observed.

10:20am **NS1-TuM7 Interphase Nanomechanical Properties in a Model Epoxy-Silane-Glass Composite as Revealed by Interfacial Force Microscopy**, *H. Cabibil, J.M. White,* University of Texas, Austin; *J.E. Houston,* Sandia National Laboratories; ***R.M. Winter***, S.D. School of Mines and Technology

The interfacial force microscope (IFM), a scanning probe microscope utilizing a self-balancing differential capacitance force sensor, was used to measure directly the interphase elastic and visco-elastic properties in model epoxy-silane-glass systems. Model composites were fabricated from diglycidyl ether of bisphenol F, diethyltoluenediamine and gamma-aminopropyltrimethoxysilane; an epoxy, amine curing agent, and organosilane respectively and optical silica fibers as the reinforcement and chemical sensor. The elastic modulus was determined directly from the force profiles using a contact mechanics analysis. It was found that the elastic modulus varies significantly with respect to the bulk in a 1-5 micron region surrounding the 50 micron glass fibers. The relaxation and creep response of the interphase was probed to investigate the visco-elastic response of the interphase. An organosilane-epoxy-glass system was also developed to model the interphase region and was probed with the IFM. Visco-elastic analysis of the model interphase yields storage and loss moduli. Fourier transform infrared evanescent wave spectroscopy, utilizing the fibers or a parallelepiped (the model interphase substrate) as both a waveguide and an evanescent sensor, and x-ray photoelectron spectroscopy were used to characterize the bulk and interphase chemistry of the systems. The relationship between interphase chemistry and nanomechanical properties were examined and will be discussed. The portion of this work done at Sandia, which is a multiprogram laboratory operated by Sandia Corporation - a Lockheed Martin Company, was supported by the United States Department of Energy under Contract DE-AC04-94AL85000.

10:40am **NS1-TuM8 Nanoindentation Mechanism and Surface Recovery in an Ionic Crystal Surface, MgO(100)**, ***P.F.M. Teran Arce***, *G. Andreu Riera, P. Gorostiza, F. Sanz,* Universidad de Barcelona, Spain

The atomic force microscope can be used to perform nanoindentations on surfaces. With the resulting indentation curves one is enabled to characterize at the nanometer level elastic and strength properties of materials. Furthermore, one is allowed to follow in situ the recovery of the surface after the indentation, therefore gaining insight into the processes affecting the dynamical behavior of the surface. We have carried out nanoindentations, only a few monatomic layers deep, on a semibrittle surface, MgO(100), utilizing an atomic force microscope both for indenting and imaging. Indentations were performed by scanning the piezo vertically until the tip contacts and eventually indents the surface. A force curve was recorded to characterize in situ the indentation. It was found that relative humidity, RH, plays a fundamental role in the kinetics of surface recovery after the indentation. Therefore, in order to avoid the influence of recovery processes in the measurement of cavity dimensions, indentations were carried out at 0 % RH when measuring elastic or strength properties. The force curves obtained show characteristic discontinuities associated with atomic layers being expelled by the tip penetrating the surface. Indentation curves extracted from the force plots show clearly two regions. One of them corresponds to the elastic deformation of the crystal. The other one starts with the onset of discontinuities and corresponds to plastic deformation. The Young modulus and hardness values of MgO(100) obtained from these experiments agree well with the known macroscopic values.

11:00am **NS1-TuM9 The Formation and Evolution of Pileup in Nanoscale Contacts**, ***K.F. Jarausch***, North Carolina State University; *J.D. Kiely, J.E. Houston,* Sandia National Laboratories; *P.E. Russell,* North Carolina State University

The interfacial force microscope (IFM) was used to indent and image defect free Au surfaces, providing atomic-scale experimental observations of the onset of pileup. The images and load-displacement measurements demonstrate that elastic accommodation of an indenter is followed by two stages of plasticity. The initial stage is identified by slight deviations of the load-displacement relationship from the predicted elastic response. Images acquired after indentations showing only this first stage of plasticity

indicate that these slight load-relaxation events result in permanent deformations 0.25 to 4.0 nm deep with no evidence of pileup or orientation dependence. The second stage is marked by a series of dramatic load-relaxation events and permanent deformations 10-100+ nm deep. Images acquired following this second stage document 0.25 nm high pileup terraces which reflect the crystallography of the surface as well as the indenter geometry. Attempts to plastically displace the indenter 4-10 nm deep into the Au surface were unsuccessful, demonstrating that the transition from stage one to stage two plasticity is associated with overcoming some sort of barrier. Stage one plasticity is consistent with previously reported models of dislocation nucleation. The dramatic load relaxations of stage two plasticity, and the pileup of material above the surface, require cross-slip and appear to reflect a dynamic process leading to dislocation intersection with the surface. The IFM measurements reported here offer new insight into the nucleation, structure and evolution of the dislocations associated with the very early stages of plasticity. This work was supported by the United States Department of Energy under Sandia Contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company.

11:20am **NS1-TuM10 Measuring and Imaging Contact Stiffness Quantitatively at the Nanoscale using Force Modulation**, ***S.A. Syed Asif***, University of Florida; *K.J. Wahl, R.J. Colton,* Naval Research Laboratory

Depth-sensing nanoindentation has been widely used to measure the nanomechanical properties of materials. However, measuring quantitative mechanical properties of surfaces and thin films on a scale below 10 nm is still a problem. In this presentation we show that combining force modulation with depth-sensing nanoindentation allows measurement of the mechanical properties of materials on the sub-nanometer scale. The stiffness sensitivity of the technique is ~0.1 N/m, which is sufficient to detect long-range surface forces and locate the surface of compliant materials. The tip-surface interaction during approach to contact, asperity deformation during contact and time-dependent deformation at the atomic scale can all be studied. We also present a novel quantitative stiffness imaging technique, which can be used directly to map the mechanical properties of materials with sub-micron lateral resolution. Quantitative stiffness imaging is particularly valuable for polymers, thin films, and other nanostructured materials.

11:40am **NS1-TuM11 SFM Studies of Environmentally Assisted Detachment of Strongly Adhering Particles@footnote 1@**, ***R.F. Hariadi***, *S.C. Langford, J.T. Dickinson,* Washington State University

The production of flat surfaces is often hindered by small particles that adhere strongly to the substrate. We have undertaken a model study of the detachment of sub-micron particles via tribological interactions. Scanning force microscope, silicon nitride tips (typically about 50 nm in diameter) are used to apply stress to 10-100 nm single crystal NaCl crystallites grown on and strongly bonded to soda-lime glass substrates. In most experiments, the applied force is a combination of a compressive normal force and a lateral force, both measured simultaneously. In a time- and spatially-resolved fashion, we apply the stress and measure the response (e.g., detachment). Only the smallest particles can be detached in dry air. However, as the relative humidity (RH) is increased, the crystallites detach at considerably lower stresses. We also observe particle reattachment as a function of time and RH; all reattachments show only a fraction of the original adhesion. We model the detachment process in terms of environmentally enhanced crack growth (due to moisture); when the crack reaches a critical length that depends on particle size, catastrophic interfacial fracture follows. Numerical estimates of the necessary work of adhesion, based on a network of ions interacting via polar forces with the glass, are described. These calculations are in reasonable agreement with our data. @FootnoteText@ @footnote 1@Work supported by the NSF Surface Engineering and Tribology Program under Grant CMS-98-00230.

Nanometer-scale Science and Technology Division
Room 6C - Session NS2-TuM

Molecular Electronics

Moderator: R.J. Hamers, University of Wisconsin, Madison

8:20am **NS2-TuM1 Single Molecule Engineering: Synthesis of Individual Biphenyl Molecules on Cu (111) with STM Tip**, ***S.W. Hla***, Freie Universitat Berlin, Germany; *L. Bartels,* Columbia University; *G. Meyer, K.-H. Rieder,* Freie Universitat Berlin, Germany

In 1904, Fritz Ullmann et al. discovered the way to produce biphenyl from iodobenzene by using Cu as a catalyst. Ever since this process is known as Ullmann reaction and becomes a basic Chemistry textbook case. Due to its varsatility to use different substituted benzenes allowing large number of products and high purity results, it is widely used in lab-style synthetic chemistry. Altogether three elementary steps involve in this reaction process; iodine dissociation from iodobenzene, migration to meet two phenyl radicals and their association to form biphenyl. Here we show that we can perform all elementary steps of Ullmann reaction over single molecules in controlled manner and can synthesize individual biphenyl molecules on the Cu(111) surface for the first time by utilising various single atom and molecule manipulation techniques with a low temperature scanning tunneling microscope (STM) at 20 K. The synthesis steps involve iodine dissociation from single iodobenzene molecules with tunneling electrons and the resulting phenyl radicals were put together by laterally moving them with STM tip. The association of two phenyl radicals to form a bi-phenyl molecule was realised by simultanuously exciting them with tunneling electrons. The threshold tunneling voltage to dissociate the iodobenzene and the energy range of phenyl oscillation on Cu(111) were determined by using I-V single molecule tunneling spectroscopy.

8:40am **NS2-TuM2 Scanning Tunneling Microscopy of Conjugated Oligomers on Si(100)**, ***B. Grandidier***, *J.P. Nys, D. Stievenard, C. Krzeminsky, C. Delerue,* IEMN CNRS, France; *J.M. Raimundo, P. Frere, J. Roncali,* IMMO, Universite d'Angers, France

Conjugated oligomers have attracted considerable interest as possible molecular wires. Investigation of the interaction of these molecules with the silicon (100) surface is therefore useful to gain insight into the way the oligomers could be connected to the silicon surface. The adsorption of different oligothiophenes on silicon (100) 2x1 have been studied by scanning tunneling microscopy in ultra high vacuum. The current constant images of the oligothiophenes are strongly bias dependent and allow the determination of the adsorption sites. The reaction involves the thiophene ring with a single Si atom of the Si=Si dimer. Ab initio calculations are performed to better characterize the chemical nature of the bonding.

9:00am **NS2-TuM3 Initial Growth of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) on Au(111): A Scanning Tunneling Microscopy Study**, *I. Chizhov,* ***A. Kahn***, *G. Scoles,* Princeton University

The structure and morphology of 3,4,9,10-perylenetetracarboxylicdianhydride (PTCDA) films deposited on Au(111) surface in ultrahigh vacuum is studied via scanning tunneling microscopy (STM). In the first monolayer, PTCDA molecules form well-ordered domains with two distinct structural phases. The first phase is characterized by a "herring-bone" arrangement of PTCDA molecules similar to that of a bulk PTCDA molecular crystal. The second phase, which had not been reported so far, is characterized by a molecular arrangement in a square pattern that does not have a known bulk analog. This second phase is less dense than the first. Only the "herring-bone" phase is consistently observed in the second and subsequent layers. The crystallographic orientation of the PTCDA layers, with respect to the Au substrate as well as with respect to each other, is directly determined from the STM images. At coverages above 2 monolayers, the formation of PTCDA islands with good molecular order is observed. Transient effects related to STM-induced dynamic changes in the PTCDA molecular layer are also discussed.

9:20am **NS2-TuM4 Isolating, Imaging, and Electrically Characterizing Individual Organic Molecules on the Si(100) Surface with the Scanning Tunneling Microscope**, ***M.C. Hersam***, *J.W. Lyding,* University of Illinois, Urbana-Champaign

Molecular electronics shows great potential as an approach for fabricating nanoelectronic devices and circuits. Despite this potential, many fundamental problems remain unsolved. This paper outlines a three pronged approach that addresses key molecular electronic issues for molecules supported on STM-patterned hydrogen passivated Si(100) surfaces. First, feedback controlled lithography (FCL) has been developed

as a reliable technique for making templates of individual dangling bonds on the Si(100):H surface. FCL detects individual H desorption events while patterning, thereby compensating for variations in tip structure. When the surface is then exposed to a flux of molecules, they bind individually to the prepatterned sites. With this technique, norbornadiene and copper phthalocyanine molecules have been intentionally isolated into predefined patterns. STM images reveal intramolecular detail and suggest mechanical behavior such as molecular rotation. Secondly, using STM spectroscopy, molecules' electronic properties have been revealed. Filled states tunneling conductance maps of copper phthalocyanine molecules exhibit an enhanced density of electronic states. However, in empty states, a ring of reduced local density of states surrounds each copper phthalocyanine molecule. Further multi-bias images reveal a more complex intramolecular electronic structure that helps to differentiate among the possible binding configurations of the molecule. Finally, an all-UHV scheme for isolating and, ultimately, electrically contacting STM-patterned nanostructures has been developed that utilizes a pre-defined p-n junction on a Si(100) substrate. With STM potentiometry, the junction is easily located, allowing for efficient registration of nanostructures after intermediate processing steps. In addition, by STM patterning across the depletion region, the electrical properties of selectively deposited nanostructures can be directly evaluated when the p-n junction is biased.

9:40am **NS2-TuM5 Molecular Wires and Molecular Junctions: Tunneling, Injection and Transport***, **M.A. Ratner,*** Northwestern University **INVITED**

Molecular wires, molecular interconnect structures, molecular emission devices and, indeed, much of molecular electronics requires efficient control of charge transport processes at the molecule/electrode interface. Direct measurements on individual molecular transport junctions are beginning to appear, and will be featured in this symposium. Understanding the conductance properties of molecular junctions requires a computational model that deals effectively with both the continuum (electrode) and discrete (molecular) aspects of the issue. The problem is similar to that of chemisorption, and the Hamiltonian models discussed are also similar. Because of this discrete/continuum coupling, the molecular levels are shifted and broadened. This leads to self energies that describe the effective state densities for injection and transport. The use of Landauer type expressions then leads to specific predictions for voltage dependence conductance in the coherent regime; most measures of individual junctions reported to date indeed can be characterized in this way. For actual injection and dissipative charge transport, the Landauer model is no longer appropriate. Here considerations of typical molecular behavior arise, and at least five different charge transport mechanisms can be posited. We will discuss some aspects of these mechanisms, advantages and disadvantages for long range charge transport in molecular wires, aspects of the energy dissipation problem and the energetic control of transport by design both of the molecule itself and of the interface.

10:20am **NS2-TuM7 Self-assembled Molecular Electronics: Is the Interface Conducting?***, T. Vondrak, C.J. Cramer, **X.-Y. Zhu,*** University of Minnesota

The use of a single molecule as a 'quantum dot' or 'quantum wire' in charge transport has attracted considerable attention due to its exciting potential in future electronic devices. A number of groups have studied the electron transport in single aromatic molecules using thiol self-assembled monolayers (SAMs) on gold surfaces. A critical issue in interpreting experimental current-voltage measurements and in designing self-assembled monolayer of molecular electronics is understanding the interfacial electronic structure. We present a systematic study to address the title question. We probe both occupied and unoccupied electronic states at the interface using laser two-photon photoemission spectroscopy, in conjunction with electronic structural calculations. We choose phenyl or fluorophenyl group tethered to the metal surface at various distance in self-assembled monolayers on Cu(111). We found that, for phenyl attached to Cu via the -S- linker, the molecular LUMO can be stabilized by as much as 3 eV. This large change cannot be accounted for exclusively by polarization effects. The majority of the stabilization energy must come from direct, strong electronic coupling between the substrate and the adsorbate. Ab initio calculations on model molecules confirms this conclusion. This kind of strong electronic coupling is absent when the molecule is located at a similar distance, but weakly coupled to the surface. Thus, we may view the -S-metal linker as a conducting contact in SAMs of molecular electronics. Our result also suggests the importance of sigma states for electron transport in short molecular wires.

10:40am **NS2-TuM8 Scanning Potentiometry Studies of Charge Transport in Sexithiophene-based FETs using Conducting Probe Atomic Force Microscopy (CP-AFM)***, **K. Seshadri,*** *T.W. Kelley, C.D. Frisbie,* University of Minnesota

Investigation of charge transport mechanisms in organic semiconductors is of immense importance to development of devices such as thin film transistors and organic-based LEDs. Of particular interest is @alpha@-sexithiophene (6T), with a hole mobility high enough for flexible, "all plastic" devices. Conducting Probe Atomic Force Microscopy (CP-AFM) has been used to measure electrical transport characteristics of 6T. The semiconductor was deposited as crystals, ranging from 1 to 6 molecules (2-14 nm) in thickness and from 1-2 µm in diameter by vacuum sublimation onto SiO2/p-Si substrates, with lithographically defined Au contacts. The semiconductor crystallite grows across the gap between two electrodes, with a capacitively coupled gate electrode, so as to achieve a field-effect transistor configuration (FET). A Au-coated conducting AFM probe is brought into contact with the electrically biased 6T crystallite, and the potential is measured as a function of position. This is a scanning potentiometry experiment, involving mapping the local potential over the surface of the organic semiconductor. Mesoscopic transport measurements, in combination with AFM imaging, are a useful strategy for elucidating charge transport across grain boundaries, charge trapping, and other structure-transport relationships in organic materials.

Nanometer-scale Science and Technology Division
Room 612 - Session NS-TuA

Innovative Nanoscale Measurements

Moderator: E.T. Yu, University of California, San Diego

2:00pm **NS-TuA1 Size, Shape, Strain, and Composition Inhomogeneities of In@sub 0.5@Ga@sub 0.5@As QDs Grown by Migration Enhanced Epitaxy**, ***N. Liu***, *C.K. Shih, O. Baklenov, A.L. Holmes, Jr.,* The University of Texas at Austin

We report cross-sectional scanning tunneling microscopy (XSTM) studies of In@sub 0.5@Ga@sub 0.5@As self-assembled quantum dots (SAQD) grown using migration enhanced epitaxy (MEE). Samples were cleaved in-situ to reveal either (110) or (1-10) cross-sectional surfaces. For the 10 ML QDs, they exhibit truncated-pyramid shapes with well-defined facets on both (110) and (1-10) projections. On the (110) surface, the orientation of the facets is about 35 degrees with respect to the base of the QDs, and on the (1-10) surfaces about 25 degrees with respect to the base. The average height of the 10 ML QDs is about 10 nm, while the average base length is about 45 nm along the (110) projection and about 61 nm along the (1-10) projection. We further discovered that the In-concentration in this kind of truncated-pyramid shaped QDs is inhomogeneous. In fact the qualitative concentration contours at high concentration show an inverted triangle shape. Similarly the distribution of the lattice parameters (as determined from the STM) within and around the QD is also inhomogeneous with its inhomogeneity consistent with an inverted triangle shape of high In-concentration in the QD. Detailed analysis and possible mechanism responsible for such a concentration distribution profile will be discussed.

2:20pm **NS-TuA2 Cross-Sectional Scanning Tunneling Microscopy as a Probe of Atomic-Scale Order in MOVPE Grown GaInP@footnote 1@**, ***J. Steinshnider***, *M. Weimer,* Texas A&M University*; M. Hanna,* National Renewable Energy Laboratory

III@sub a@-III@sub b@-V alloys grown by metal-organic vapor phase epitaxy (MOVPE) exhibit varying degrees of CuPt-B order in which III@sub a@ and III@sub b@ atoms preferentially enrich alternating -B planes during growth to form a monolayer superlattice. We have used cross-sectional scanning tunneling microscopy (STM) to examine and characterize spontaneous ordering in MOVPE-grown GaInP films lattice-matched to GaAs. We show how cross-sectional STM permits the direct, real-space visualization of CuPt order based on III@sub a@-III@sub b@ site discrimination, and indicate how the degree of local order in selected regions of a sample may be quantitatively assessed through the In-In pair correlation function constructed from atomic-resolution data. We introduce a local order parameter, based on the pair correlation function, that is identified with the Bragg-Williams parameter in the case of long range order and which allows a direct comparison of the STM results with optical or x-ray measurements. We have examined the spatial evolution of the local order parameter in the vicinity of the alloy / buffer interface, where the STM images show evidence for atomically-abrupt antiphase boundaries, and find that the onset of recognizable group-III sublattice order requires approximately twenty monolayers. The ability of cross-sectional STM to probe the development of local order on these length scales suggests it will be a powerful tool for studying the mechanism of atomic ordering as well as optimizing the growth of ordered films. @FootnoteText@ @footnote 1@Work supported in part by a grant from the National Science Foundation, Division of Materials Research.

2:40pm **NS-TuA3 Interpreting Atomic-Scale Structure in Cross-Sectional STM Images of III-V Superlattices**, *W. Barvosa-Carter,* ***B.Z. Nosho***, *M.J. Yang, L.J. Whitman,* Naval Research Laboratory

Cross-sectional scanning tunneling microscopy (XSTM) is a powerful method for quantifying the structural and interfacial quality of III-V semiconductor superlattice structures. Although a variety of III-V systems have been studied with XSTM, there are a number of aspects related to image interpretation, particularly on the atomic-scale, that are still a matter of discussion. One rarely discussed issue is that on the (110) cleavage face only every other III-V growth layer within the superlattice can be directly observed by XSTM. This fact can have important consequences when investigating properties of the superlattice such as the roughness between heteroepitaxial layers, interfacial defects, or variations in chemical bonding at the interface. The impact is especially significant when these effects occur predominantly within a volume only two to three monolayers (ML) wide. We are systematically investigating the appearance of III-As and III-Sb bonds at arsenide-antimonide interfaces as a function of cleavage direction and even-versus-odd layers in specially prepared MBE-grown superlattices. We find it is possible to differentiate between the two bond types, but their appearance depends on cleavage-face and layer order. In addition, a model of the measurement of interfacial roughness reveals errors in the measured power spectrum as the actual interface roughness decreases below 2 ML. A simple method for reconstructing the actual power spectrum from the STM data will be described. Funded by the Office of Naval Research and the Air Force Research Laboratory. Present address for W. Barvosa-Carter is HRL Laboratories, Malibu, CA.

3:00pm **NS-TuA4 The Importance of Many-body Effects in the Clustering of Charged Zn Dopant Atoms in GaAs**, ***Ph. Ebert***, Forschungszentrum J@um u@lich, Germany*; T.-J. Zhang,* University of Tennessee*; F. Kluge, M. Simon,* Forschungszentrum J@um u@lich, Germany*; Z. Zhang,* Oak Ridge National Laboratory*; K. Urban,* Forschungszentrum J@um u@lich, Germany

The spatial distribution of negatively charged Zn dopant atoms in GaAs has been investigated by cross-sectional scanning tunneling microscopy. At high densities, the dopant atoms exhibit clear clustering behavior, suggesting the existence of an effective attractive interaction in addition to the screened Coulomb repulsion between two dopants. By analyzing the data through Monte Carlo simulations, we have extracted the intrinsic screening length at different dopant densities, and attributed the origin of the effective attraction to strong many-body effects in the dopant-dopant repulsion.

3:20pm **NS-TuA5 New Methods to Measure Electrical, Optical, and Magnetic Properties on the Nanometer Scale**, ***M. Aono***, Osaka University and Institute of Physical and Chemical Research, Japan **INVITED**

In order to measure electrical, optical, and magnetic properties of materials on the nanometer scale, we have developed (a) a scanning tunneling microscope (STM) that has three tips operated independently, (b) a photon-detecting STM equipped with a polari zation analyzer, and © a spin-polarized STM with a nonmagnetic high-Z material tip, respectively. In the present paper, we show selected experimental results obtained with these apparatuses. Also we would like to show interesting experimental results on local polymerization of organic molecule in monolayer films. They include chain polymerization of diacetylene compound molecules triggered by a STM tip.

4:00pm **NS-TuA7 Field Dependent Electric Potential Gradients at Atomically Abrupt Oxide Interfaces**, ***D.A. Bonnell***, *B. Huey, S. Kalinin,* University of Pennsylvania

Scanning Surface Potential Microscopy has been used to measure spatial variations in electric fields near atomically abrupt interfaces in SrTiO@sub 3@ and ZnO. The field dependence of potential gradients is determined by using microlithography to isolate regions of the interface and apply local electric fields during the measurements. The local potential drop is used to determine the interface density of states. A procedure for extracting actual interface potential from separation dependence is proposed.[100] symmetric tilt boundaries in SrTiO@sub 3@ with tilt angles ranging from 15°-60° are examined and interface potential is related to atomic structure.

4:20pm **NS-TuA8 Dynamics of Adsorbate Islands with Nanoscale Spacial Resolution: (OH)@sub n@ Formation during the NO/H@sub 2@ Reaction on Pt(001)**, *C. Voss, T. Visart de Bocarmé, T. Bär,* ***N. Kruse***, Université Libre de Bruxelles, Belgium

Studies by Field Ion Microscopy (FIM) of the catalytic NO hydrogenation (p@sub H2@ = 4 x 10@super -3@ Pa and p@sub NO@ = 3 x 10@super -3@ Pa at 500 K) on the (001) plane of a Pt tip have resulted in the observation of small islands with a size corresponding to 10-30 Pt surface atoms. Simultaneous atom-probe work allowed these islands to be consistently interpreted as being due to the intermediate formation of hydroxyl species in an O@sub ad@/H@sub ad@ coadsorbed layer. Imaging of this reaction phenomenon was achieved by field ionisation of NO at field strengths slightly above those usually present in Scanning Tunneling Microscopy (STM). OH@sub ad@ islands exclusively formed at the layer edge with subsequent movement into the (001) terrace region. Usually one to two islands were observed at the same time with no mergence occurring on collision. Mean lifetimes of several minutes were observed for individual islands before their annihilation at the layer edge. The formation of OH@sub ad@ clusters must be regarded as a collective reaction phenomenon involving a delicate balance of attractive and repulsive forces between adspecies. The results will be presented in a video sequence and compared to a sucessful computer simulation with an automaton lattice model.

4:40pm **NS-TuA9 Measuring Average Tip-sample Forces in Intermittent-contact (Tapping) Force Microscopy in Air**, ***S.C. Fain, Jr.,*** *K.A. Barry, M.G. Bush, B. Pittenger,* University of Washington*; R.N. Louie,* Pacific Lutheran University

Many soft substances such as polymers and biological molecules show much less damage when imaged with intermittent-contact (tapping) force microscopy; however, the tip-sample forces involved have never been directly measured. The mathematical solutions to the non-linear differential equations needed to calculate these forces can be extremely complicated even for mass-on-a-spring models. In these experiments piezoresistive cantilevers (from Park Scientific/ ThermoMicroscopes) are used to measure the average force on a silicon surface produced by the silicon tip of a separate mechanically-driven (active) cantilever. The procedure consists of slowly moving the two cantilevers toward and away from each other while measuring as a function of the change in distance between the two support points: the average deflection of the piezoresistive cantilever, the amplitude of the active cantilever, the change in phase of the active cantilever relative to the mechanical driver, and the change in the average deflection of the active cantilever. Recent simulations by Garcia and San Paulo (Phys. Rev. B., in press) predict the force exerted on a model substrate averaged over a complete cycle, the amplitude, and the phase shift as a function of distance; they find that the force starts to rise when the phase shift indicates repulsive tapping. These predictions are compared with our measurements. The limit on the sensitivity of our average force measurements is set by the 1/f noise of the piezoresistive cantilever. This work was supported by NSF DMR 96-23590 and the UW Royalty Research Fund.

5:00pm **NS-TuA10 Imaging the Near-field Intensity Gradients with a Tapping-mode Near-field Scanning Optical Microscope**, ***D.P. Tsai,*** *C.W. Yang,* National Chung Cheng University, Taiwan

A tapping-mode near-field scanning optical microscope system using a non-optical tuning fork method has been developed recently. One of the advantage of this new method is that tapping of the near-field optical fiber probe can provide the measurements of the near-field intensity gradients at different heights vertically. Based on the modulation of the near-field optical fiber probe, near-field intensity gradients were used as a new contrast mechanism of the NSOM. The imaging of the near-field field optical intensity gradients have been successfully applied on the study of both the propagating and evanescent field intensity. The propagating field with a constant intensity shows an image of zero gradients. The evanescent intensity gradients of the configurations of total international reflection or surface plasmons, on the other hand, indicate the local optical properties of the photon-matter interactions. Imaging contrast of the near-field optical intensity gradients of a focused spot on the clear cover glass slip and the gold-coated cover glass slip will be shown. Property of the local optical interactions of the gold thin film in near field was discerned. Results demonstrate the novelty of the imaging contrast of the near-field intensity gradients.

Electronic Materials and Processing Division
Room 6C - Session EM+NS-WeM

Nano-characterization of Molecules, Materials, and Devices

Moderator: R.S. Goldman, University of Michigan

8:20am **EM+NS-WeM1 Homoepitaxy on AlSb(001): Novel Reconstructions and Their Implications for Nucleation and Growth**, ***W. Barvosa-Carter,*** HRL Laboratories*; A.S. Bracker, J.C. Culbertson, B.V. Shanabrook, B.R. Bennett, L.J. Whitman,* Naval Research Laboratory*; N. Modine,* Sandia National Laboratories*; H. Kim, E. Kaxiras,* Harvard University

Strained-layer heterostructures involving the 6.1 Å family of III-V semiconductors (InAs, GaSb, and AlSb) are being investigated for use in a growing number of high-frequency and infrared devices. The structure of the interfaces in these heterostructures can be critical to device performance, and device optimization will ultimately require precise and reproducible control over surface morphology during growth. To accomplish this level of morphological control, models are being developed which relate process parameters to surface roughness. These models require a detailed understanding of the relevant surface reconstructions and the mechanisms by which epitaxy proceeds. Using MBE, RHEED, and STM (performed at NRL), combined with first-principles theoretical calculations, we have discovered a novel (4x3) reconstruction on the nominally "(1x3)" AlSb(001) growth surface. This new reconstruction is different than those previously proposed for this surface and, surprisingly, includes mixed III-V dimers in the top layer of the reconstruction. The presence of surface Al atoms close to their natural lattice sites leads to nucleation and growth mechanisms that are fundamentally different than for III-As systems. We have also studied AlSb homoepitaxy as a function of coverage. The relationship between the observed reconstructions, island structure, island distributions, and possible growth modes will be discussed.

8:40am **EM+NS-WeM2 A New Point Projection Microscope for the Holographic Imaging of Single Macromolecules**, ***A. Eisele,*** *B. Völkel, A. Glenz, B. Jäger, A. Gölzhäuser, M. Grunze,* Universität Heidelberg, Germany

In Low Energy Electron Point Source microscopy the spatial coherence of electrons from point sources can be utilized to image single molecules. A molecular object is positioned ~100 nm in front of the source and interference patterns between the part of the electron's wave function that scatters at the object and the part that passes by unscattered are recorded.@footnote 1@ Structural information on the molecule can then be obtained by numerical reconstruction of the hologram.@footnote 2,3@ We have built a new microscope for the recording of holograms at high magnification (@>=@10@super 6@) and under the minimization of critical disturbances like vibrations and alternating magnetic fields. In the presented instrument projection microscopy can be interleaved with in-situ preparation of the source via field emission / field ion microscopy. The microscope has been tested by the imaging of single DNA molecules that were deposited on thin structured siliconmembranes. Numerical reconstructions of the obtained holograms show corrugated strands with a diameter of ~2 nm. @FootnoteText@ @footnote 1@ H.-W. Fink, W. Stocker, and H. Schmid, Phys. Rev. Lett. 65, 1204 (1990) @footnote 2@ H. J. Kreuzer, K. Nakumura, A. Wiezbicki, H.-W. Fink, and H. Schmid, Ultramicroscopy 45, 381 (1992) @footnote 3@ A. Gölzhäuser, B. Völkel, B. Jäger, M. Zharnikov, H.J. Kreuzer, M. Grunze, J. Vac. Sci. Technol. A16(5), 3025 (1998)

9:00am **EM+NS-WeM3 Single Molecule Vibrational Spectroscopy with a Variable Temperature STM**, ***L.J. Lauhon,*** *W. Ho,* Cornell University **INVITED**

The ultimate sensitivity for vibrational spectroscopy is the detection of a single bond. The vibrational spectrum of a single molecular adsorbate carries information about the effects of the local environment on chemical bonding. Such effects are the basis of important processes such as catalysis. Single bond sensitivity was recently demonstrated by using a scanning tunneling microscope to perform inelastic electron tunneling spectroscopy (STM-IETS) on a single acetylene molecule.@footnote 1@ We have extended this technique to other molecules at temperatures from 8 K to 60 K in an effort to both better understand and widen the applicability of STM-IETS. Two 'tunneling-active' vibrational modes have been identified for CO adsorbed on Cu(001) and Cu(110). The effects of monatomic steps and coadsorbed potassium on the vibrational spectra, including peak shifting and quenching, were found to be local in nature. The increase in the vibrational peak width with temperature was measured up to 40 K, beyond which thermal diffusion prevented STM-IETS spectra from being recorded. STM-IETS was also performed on pyridine and benzene adsorbed on Cu(001). Though these molecules differ only in the substitution of a nitrogen atom for one C-H group, their bonding geometries and vibrational spectra are very different. Achieving the spatial limit of nanotechnology depends on the ability to perform chemistry on the atomic scale. To this end, tunneling electrons were used to dissociate individual pyridine and benzene molecules. The adsorbtion geometries of the reaction products differ from the parent molecules and lead to changes in the vibrational spectra which provide insights into the identities of the reaction products and the tunneling mechanism. The extension of STM-IETS to new functional groups, including larger molecules, will also be discussed. @FootnoteText@ @footnote 1@ B. S. Stipe, M. A. Rezaei, and W. Ho, Science Vol. 280, p. 1732 (1998).

9:40am **EM+NS-WeM5 Characterization of Electronic Materials and Devices by Scanning Probe Microscopies**, ***C.C. Williams,*** *V. Zavyalov, L. Klein,* University of Utah*; J. Kim,* Korea Advanced Institute of Science and Technology **INVITED**

Several studies of the electrostatic properties of oxides and silicon devices have been performed by the Scanning Capacitance Microscope (SCM) and the Electrostatic Force Microscope (EFM). The SCM provides a method for measuring topographical and electrical roughness of thin oxides, surface charge and local carrier and dopant density in semiconductors. On thin oxides, the SCM reveals a nanometer scale variation in the "electrical thickness" of the oxide. The thickness variations seen by SCM have been compared with topographical (AFM) and surface potential measurements by EFM in UHV. Surface potential variations of order 5 mV are observed on the same spatial scale as the thickness variations seen by the SCM. Calculations show that the measured surface potential variations correspond to less than one electron per tip area (30 nm radius). Single MOSFET devices have been imaged in cross-section under active electrical bias by SCM. The images provide a measure of the distribution of the carriers in a device under bias. Finally, a new technique will be described for detecting the transfer of a single electron between a SPM tip and surface.

10:20am **EM+NS-WeM7 Mapping Composition and Electrostatic Potential in Devices**, ***A. Ourmazd,*** *A. Orchowski, W.-D. Rau, P. Schwander,* IHP, Germany **INVITED**

An electronic device is, in essence, a microscopically varying electrostatic potential surface, which steers the charge carriers between the device's terminals. Until recently, there were no means for directly measuring the electrostatic potential distribution in the bulk of devices. It is now possible to map the electrostatic potential in two dimensions by electron holography. Maps of deep submicron transistors have been obtained with nanometer spatial resolution and 0.1V sensitivity. The electrostatic potential surface can be tailored by changes in composition and/or doping. It is often important to separate the two effects. Electron holography alone, however, cannot distinguish between them; they both change the electrostatic potential. QUANTITEM, on the other hand, is sensitive to compositional changes only. Efforts are under way to combine the results from electron holography and QUANTITEM, in order to separate the effects of composition and doping, with first encouraging results.

11:00am **EM+NS-WeM9 Failure Analysis of Sub 1/4-Micron Contacts by Means of TEM-EELS**, ***F. Yano,*** *Y. Nakamura, T. Aoyama, Y. Mitsui,* Hitachi Ltd., Japan

Although TEM-EELS (Transmission Electron Microscope-Electron Energy Loss Spectroscopy) has practically been used for elemental analysis for nanometer area, its full potential, we believe, is achieved when it is used for chemical analysis just like ESCA. This paper uncovers our experience of thermally stable contact development, in which our advanced TEM-EELS@footnote 1@ has revealed reactions in the contact during thermal process, which have detrimentally increased its resistivity.@footnote 2,3@ The contact holes are filled with sputtered Ti, which is annealed to form TiSi@sub 2@, CVD-TiN and CVD-W. Alathough the contact resistivity was low enough just after contact processes, it became higher after thermal process. The resistivity was varied 10@super 2@ to 10@super 6@ @ohm@ depending on the process conditions. Chemical analysis of loss energies showed that Si substrate in the contact is fully covered with SiO@sub 2@ in the fatal worst case. Even somewhat better cases, TiSi@sub 2@ formation was partial and still SiO@sub 2@ was formed. In other cases, TiO@sub x@ was also observed. These oxidized layers clearly increased resistivity. However, the mechanism of oxidation was unclear,

especially the origin of the oxygen was, because neither oxygen nor water was applied. To clarify the mechanism, we made a model, in which residual TiCl@sub x@ on CVD-TiN forms titanium acid gel (TiO@sub x@(H@sub 2@O)@sub n@) which works as a water reservoir. During thermal process, the water in the gel is released, which goes through TiN grain and finally oxidizes silicon at the interface of TiN and Si substrate. To prove this model, the relation between the amount of residual Cl and the contact resistivity was measured. The results supported the model above, i.e., the more Cl observed, the higher the resistivity is. Based on this mechanism, all cases of high resistivity failures in the thermally stable contact were explained. Chemical analysis by TEM-EELS will be a key technique for failure analysis of 1/4-micron devices and after. @FootnoteText@ @footnote 1@ T. Sekiguchi, et al., Jpn. J. Appl. Phys., vol. 37 (1998) L694. @footnote 2@ Y. Mitsui, et al., Ext. Abst. IEDM (1998) 329.@footnote 3@ Y. Nakamura, et al., Proceedings of Advanced Metallization Conference, Colorado (1998) 661.

11:20am **EM+NS-WeM10 Applications of AFM/SCM in Imaging Implant Structures of Semiconductor Devices**, ***K.-J. Chao****, J.R. Kingsley, R.J. Plano, X. Lu, I.D. Ward,* Charles Evans & Associates

The scanning capacitance microscopy (SCM) has been widely used to investigate the two-dimensional carrier profile of semiconductor devices. In this work, SCM is used to investigate several different semiconductor devices. First, one commercially purchased integrated circuits (IC) device was cross-sectioned and polished for the SCM investigation. Implant structures near the gate were clearly resolved. Second, two semiconductor devices, one was good and the other was failed, were prepared by cross-sectioning and then followed by polishing. Implant profiles of similar structures on both devices were revealed by SCM. As compared with the good device, the thickness of the N-well structure was found to be thinner by about 0.4um for the failed device. Third, a GaAs device with Zn thermally diffused through the Si3N4 mask was studied to determine the lateral diffusion length of Zn. Applications in other cases will be presented at the conference.

11:40am **EM+NS-WeM11 Capacitance Measurements on Gold Nanowires**, ***A. Wlasenko****,* McGill University, Canada

There are several assumptions made about classical capacitors (C=Q/V): the density of states(DOS) of the plates is infinite, the potential drop occurs entirely across the plates, electrons don't interact, and there is no tunnelling. In mesoscopic capacitors, the voltage drop doesn't occur entirely across the plates, and the finite DOS plays an important role. In the experimental setup presented, the voltage-dependence of C is measured for gold nanowires allowing the DOS to be deduced according to theory [H. Guo et al., APL 74, 2887-2889 (1999)]. A piezotube is used to retract a gold sample in contact with a gold tip to form a nanowire. Along with measurements of C, simultaneous measurements of conductance(G) are made with a current preamplifier to monitor the transmission properties of the contact. Changes in the C of this nanowire are measured by a modified RCA Video Disc sensor: a resonant circuit is connected to a 915 MHz oscillator, and the amplitude of the signal is measured. A change in C leads to a shift in the resonance peak which is detected by the sensor. The sensor is calibrated using a ball bearing and metal plane geometry in comparison with classical calculations. The sensor is sensitive to C changes as low as 10@super -17@ F. When the tip and sample are in contact, the sensor measures a convolution of C and G. Where a variation in C leads to a shift in the resonance peak, a variation in G leads to a change of the FWHM. Measurements on either side of the resonance peak can be made in order to seperate C and G.

Nanometer-scale Science and Technology Division
Room 612 - Session NS-WeM

Nanopatterning

Moderator: C.R.K. Marrian, Naval Research Laboratory

8:20am **NS-WeM1 "MILLIPEDE" - A Highly Parallel, Very Dense AFM-Based Data Storage System**, ***P. Vettiger****, M. Despont, U. Drechsler, U. Dürig, W. Häberle, M.I. Lutwyche, H. Rothuizen, R. Stutz, R. Widmer, G.K. Binnig,* IBM Research Division, Zurich Research Laboratory, Switzerland **INVITED**

We report on an alternative storage approach based on scanning probe techniques having areal density potential far beyond and data rates comparable to today's magnetic-recording techniques.@footnote 1,2@ Ultra-high areal density is achieved by thermomechanical writing/reading in very thin polymer films, and the high data rate by highly parallel operation of very large, 2D cantilever/tip arrays.@footnote 2@ Potential for ultra-high density was demonstrated by 40-nm bit indents and 40-nm bit pitch in 50-nm-thick polymers films (PMMA), resulting in 400 Gbit/sq inch.@footnote 3@ We also demonstrated, for the first time, large area thermal data erasing/rewriting in such polymer films. First functional 32x32 (1024) cantilever array chips were fabricated,@footnote 4@ which are among the densest VLSI-NanoEMS chips. The 32x32 array is fabricated on an 3x3 mm area of a 7x14-mm silicon chip. Four integrated approaching/leveling sensors in the four corners control the simultaneous approach of the entire chip. While the feedback control system keeps the chip leveled and the tips in contact with the media, the media is scanned in the X and Y directions. Writing/reading is controlled by a time-multiplexed row/column addressing scheme. Similar micromaching techniques were used to fabricate a silicon micromagnetic X/Y/Z scanner with integrated Cu coils.@footnote 5@ We present details on the MILLIPEDE storage concept, the thermomechanical write/read/erase processes/results as well as the VLSI-NEMS chip and micromagnetic X/Y/Z scanner fabrication. @FootnoteText@ @footnote 1@ H.J. Mamin et al., IBM J. Res. Develop. 39, 681 (1995). @footnote 2@ P. Vettiger et al., Proc. Int'l Conf. on Micro- and Nanoengineering 98, Leuven, Belgium, Sept. 1998, to appear in J. Microelectron. Eng. @footnote 3@ G. Binnig et al., Appl. Phys. Lett. 74, 1329 (1999). @footnote 4@ M. Despont et al., Technical Digest MEMS'99, p. 564 (IEEE, 1999). @footnote 5@ M. Lutwyche et al., Proc. 194th ECS Mtg., Boston, MA (in press).

9:00am **NS-WeM3 Scanning Probe Lithography of Silicon Nitride Thin Films**, ***F.S.-S. Chien****,* National Chiao Tung University, Taiwan*; S.W. Lin,* National Tsing Hua University, Taiwan*; W.-F. Hsieh,* National Chiao Tung University, Taiwan*; Y.-C. Chou, T.-T. Chen,* National Tsing Hua University, Taiwan*; T.S. Chao,* National Nano Device Laboratory, Taiwan*; S. Gwo,* National Tsing Hua University, Taiwan

Silicon nitride has been extensively used as etch stops, diffusion barriers, oxidation masks, and gate dielectric layers in integrated circuit processing. A new method is proposed here to perform local oxidation and negative pattern transfer on silicon nitride thin films. A LPCVD silicon nitride film of 25 Å thickness grown on a p-type silicon wafer is locally oxidized by the probe of an atomic force microscope under positive biases of 5 V to 10 V. In this approach, nanometer-size oxidation patterns can be made on the silicon nitride film. By using the selective HF etching, the oxidized regions on the silicon nitride film can be removed. In a second step, the orientation dependent KOH etching, which has an extremely large selectivity between silicon and silicon nitride, can produce high-aspect-ratio trenched structures (pattern transfer of the original oxide mask) on the (110)-oriented silicon wafer. Such a new method of producing negative-resist pattern tranfer can greatly enhance the capabilities of scanning probe lithography for the future microelecronics and optoelectronics applications on the nanometer scale. @FootnoteText@ F. S.-S. Chien is also with Center for Measurement Standards, Hsinchu, Taiwan.

9:20am **NS-WeM4 Nanolithography and Pattern Transfer of (110)-oriented Silicon Using Scanning Probe Lithography and Anisotropic Wet Etching**, ***C.-L. Wu****,* National Tsing Hua University, Taiwan*; S.-S. Chien, W.-F. Hsieh,* National Chiao Tung University, Taiwan*; T.-T. Chen, Y.-C. Chou, S. Gwo,* National Tsing Hua University, Taiwan

Recently, scanning probe lithography has became an emerging technology capable of fabricating sub-micron structures. We have demonstrated that silicon nanostructures (~60 nm lateral dimension) with high aspect ratios and large structural heights (~400 nm) may be fabricated by scanning probe lithography and aqueous KOH orientation-depentent etching on the H-passivated (110)Si wafer. The High spatial resolution of fabricated features is achieved by atomic force microscope based nano-oxidation process in ambient and anisotropic selective wet etching. Combining the large (110)/(111) anisotropic ratio of etch rate and large Si/SiO@sub2@ etch selectivity of aqueous KOH etching at an optimal concentration and a relatively low etching temperature, structural ridges of high-aspect-ratio and excellent parallelism as well as a hexagonal pit structure determined by the terminal etch geometry can be obtained. This method is potentially useful for simple and reliable high-packing-density and high-aspect-ratio micromachining on the nanometer scale.

9:40am **NS-WeM5 Patterning of Silicon Surfaces With a Non-Contact Atomic Force Microscope: Attomol Chemistry and Nanofabrication**, ***R. Garcia****, M. Calleja,* Consejo Superior Investigaciones Cientificas, Spain*; H. Rohrer,* Switzerland

Nanometer-size water bridges have been used to confine the anodic oxidation of silicon surfaces with a non-contact atomic force microscope.

The formation of a water bridge between two surfaces separated by a gap of a few nanometers is driven by the application of an external electrical field. Once a liquid bridge is formed, its length and neck diameter can be modified by changing the tip-sample separation. The liquid bridge provides the ionic species and the spatial confinement to oxidize Si(100) surfaces.@footnote 1,2@ The very small number of active ionic species within the bridge, a few attomoles, allows a precise control of the lateral and vertical size of the oxide. Above results are applied to develop a highly reproducible method to nanofabricate two types of patterns: (i) arrays of 5000 dots with a periodicity of 40 nm and an average width of 10 nm and (ii) lines 10 micron long and 10 nm wide. @FootnoteText@ @footnote 1@R. Garcia, M. Calleja and F. Perez-Murano, Appl. Phys. Lett. 72, 2295 (1998). @footnote 2@R. Garcia, M. Calleja and H. Rohrer, J. Appl. Phys. (in press).

10:00am **NS-WeM6 Fabrication of Nanoscale Metal Wires on the Si(001) Surface Using Scanning Tunneling Microscopy**, ***T. Mitsui***, *E. Hill, R. Curtis, E. Ganz,* University of Minnesota

Nanoscale wires are fabricated on the Si(001)-(2x1) surface using an atomic hydrogen resist process.@footnote 1@ The patterning is achieved by removing small areas of the hydrogen passivation layer with a scanning tunneling microscope. Pattern transfer is performed by chemical vapor deposition (CVD) or physical vapor deposition (PVD). CVD provides higher selectivity than PVD. However, Ti selective CVD growth from TiCl@sub 4@ is self limiting by Cl passivation. Growth can be resumed by removing the Cl passivation locally using the STM. Al selective CVD produces 3 nm wires although the wires appear to be granular and sequential growth roughens the pattern. To improve the wire quality, we are now using selective Pd silicide growth by PVD. @FootnoteText@ @footnote 1@T-C. Shen, C. Wang, G. C. Abeln, J. R. Tucker, J. W. Lyding, Ph. Avouris, and R. E. Walkup, Science 268, 1590 (1995).

10:20am **NS-WeM7 Growth and Characterisation of Submicrometer Regular Arrays of Pillars and Helices**, ***M. Malac***, *R.F. Egerton, M.J. Brett,* University of Alberta, Canada

The fabrication of photonic bandgap structures presents one of the current challenges in microfabrication. Submicron periodic structures with a high aspect ratio are necessary to create a structure with a photonic bandgap in the visible or near infrared region. We have fabricated arrays of pillars and helices with lattice parameter down to 300nm and aspect ratio as high as 25. We utilize oblique-angle deposition onto a rotating substrate (GLAD technique) to grow our films. A square array with lattice parameter between 300 nm and 1 micrometer was patterned onto the substrate prior to film growth. The array was made using electron beam lithography based on PMMA resist followed by lift-off. The array provides preferential sites for shadowed film growth when the film is deposited onto a substrate which is oblique with respect to the arriving species. This method provides a high degree of process control and sufficient number of degrees of freedom to allow for the growth of a wide range of structures. Our microstructures were made of titanium or bismuth, chosen for the large difference in their melting points. All films were deposited onto a room-temperature substrate, implying a low adatom diffusion length for titanium (due to a low ratio of substrate temperature and melting point) but a large adatom diffusion length for bismuth (where bulk diffusion may play a significant role). The titanium pillar structures appear to be uniform along their length, the crystallite size being smaller than the pillar diameter. Regular arrays of titanium helices exhibited bifurcation within each helix, whereas bifurcation was strongly suppressed in both helices and pillars made of bismuth. The delibrate introduction of a defect into the patterned array did not have a radical effect on film growth.

10:40am **NS-WeM8 Plasma Polymerization as a Novel Means of Preparing Concentric-Tubular Composite Microstructures**, ***E.R. Fisher***, *M.L. Steen, J.R.D. Peers,* Colorado State University

Template synthesis has been shown to be a general method for preparing micro- and nanostructured materials. This method entails synthesizing a desired material in the pores of microporous filtration membranes. Concentric-composite micro- and nanostructures have also been prepared by the template method. Such concentric-tubular structures consist of an outer tubule of one material surrounding inner tubules of different materials. Synthetic methodologies for preparing concentric-tubular micro- and nanostructures include electroless deposition of Au, electropolymerization of metals and semiconductors, carbonization of polymer precursors, chemical-vapor deposition and sol-gel synthesis. Thus, these methodologies are used to prepare composite micro- and nanostructures composed of metals, semiconductors, carbon, polymers and Li@super +@-intercalation materials. We propose an alternative synthetic methodology to preparing concentric-tubular micro- and nanostructures of this type. This method employs plasma polymerization to deposit polymeric conformal coatings on Au micro- and nanotubules synthesized by the template method. There are several experimental advantages to using plasma polymerization. Polymer-formation occurs from almost all volatile organic molecules, even those lacking vinyl and aromatic groups necessary for other polymerization schemes. The chemical composition of the deposited films can be controlled by adjusting plasma parameters, such as applied rf power, monomer flow rate, and pulsed vs. CW conditions. An extensive parameter study of several plasma systems has been examined. We have prepared several Au-insulating and Au-conducting polymer concentric-composite micro- and nanostructures by plasma polymerization. For example, polystyrene-coated Au microstructures are obtained from a pulsed benzene plasma. Results from scanning electron microscopy and electrochemical characterization will be discussed.

11:00am **NS-WeM9 Fabrication of Bismuth Nanowires with a Silver Nanocrystal Shadowmask**, ***S. Choi***, *K. Wang,* University of California, Los Angeles*; M. Leung, G. Stupian, N. Presser, B. Morgan, R. Robertson, E. King, M. Tueling,* Aerospace Corporation*; S. Chung, J. Heath,* University of California, Los Angeles*; S. Cho, J. Ketterson,* Northwestern University

There has been much interest in arrays of bismuth (Bi) nanowires for both fundamental understanding and device application because of many interesting properties such as long mean free path of the carriers and the small effectiveness and the semimetal-semiconductor transition. In this abstract, we describe a method of using silver (Ag) nanocrystal wires as a shadowmask to produce nanometer-size Bi wire patterns and discuss transport properties of Bi nanowires. In our technique, organically functionalized Ag nanocrystals (2-100nm) can assemble into lamella (wire-like) phases. The width of the wires could be controlled from 20 to 300nm. The wire patterns can be transferred as Langmuir-Scheffer (horizontal lift-off) films to the polymethyl methacrylate (PMMA) coated Bi/CdTe substrates. Bi epilayers were grown by molecular-beam epitaxy (MBE) on CdTe (111) B substrates. X-ray diffraction showed only sharp (00.l) peaks were present, which implied c-axis growth of Bi perpendicular to the substrates. Cleanness of surface of Bi films was also confirmed by the Time-Of-Flight Secondary Ion Mass Spectroscopy (TOFSIMS) using high energy Gallium ions. The wire patterns were transferred to the PMMA films by spatially selective electron beam exposure on the Ag nanocrystal wire shadowmask. 50 nm and 70 nm wide Bi wire patterns were formed by a subsequent anisotropic reactive ion etching (RIE) process. The metal contacts on the Bi nanowires were prepared by in-situ Focused Ion Beam (FIB) deposition for temperature dependent resistance measurement. In zero magnetic field, the temperature dependent resistance measurements on the Bi nanowires with widths of 50 nm and 70 nm showed the resistance increased with decreasing temperature, which was characteristic for semiconductor and insulators.

11:20am **NS-WeM10 Fabrication of Metal Nano-wires using Carbon Nanotube Masks**, ***W.S. Yun***, Seoul National University, Republic of Korea*; K.-H. Park, J.S. Ha, K. Park,* ETRI, Republic of Korea*; J. Kim,* KRISS, Republic of Korea*; S.K. Kim,* Seoul National University, Republic of Korea*; J.-P. Salvetat, L. Forró,* EPFL, Switzerland

Circumventing problems lying in the conventional lithographic techniques, we devised a new method for the fabrication of nanometer scale metal wires using the unique characteristics of carbon nanotubes (CNTs). Since carbon nanotubes could act as masks when CNT-coated thin Au/Ti layer on a SiO@sub 2@ surface was physically etched by low energy argon ion bombardment (ion milling), Au/Ti nano-wires were successfully formed just below the CNTs exactly duplicating their lateral shapes. Cross-sectional analysis by transmission electron microscopy revealed that the edge of the metal wire was very sharply developed indicating great difference in the milling rates between the CNTs and the metal layer as well as the good directionality of the ion milling. We could easily find a few nanometer-wide Au/Ti wires among the wires of various widths. After the formation of nano-wires, the CNTs could be pushed away from the metal nano-wire by atomic force microscopy. The lateral force for the removal of the CNTs is dependent upon the width and shape of the wires. Resistance of the metal nano-wires without the CNTs was also measured through the micro-contacts defined by electron beam lithography. Since this CNT-based lithographic technique is, in principle, applicable to any kinds of materials, it can be very useful in exploring the fields of nano-science and technology, especially when it is combined with the CNT manipulation techniques.

11:40am **NS-WeM11 Strain Effects on the Growth Modes at Stepped Surfaces**, ***D.Y. Petrovykh***, *J.-L. Lin, J. Viernow, A. Kirakosian, A. Li, F. Liu, M.G. Lagally, F.J. Himpsel,* University of Wisconsin, Madison

Strain and atomic steps have been used previously to control size, spacing and alignment of self-assembled nanostructures. In this study we utilize high quality Si(111) stepped surfaces as templates for growth of CaF@sub 2@ nanostructures.@footnote 1@ The growth modes in this system in the submonolayer coverage regime are strongly influenced by strain. The step flow mode is expected for deposition rates and substrate temperatures used in our experiments. Instead the growth results in strings of islands attached to step edges. Only for coverage around 0.5 monolayer and above we observe continuous stripes characteristic of the step flow mode. The above two regimes may be beneficial for self-assembly of quantum dot and wire arrays respectively. It has been recently suggested@footnote 2@ that the misfit strain is responsible for the initial roughening of the growth front and formation of islands. Beyond a critical coverage the roughening is suppressed by the interaction between islands on adjacent terraces and continuous stripes become more favorable. A quantitative comparison of experimental results with theory is presented. @FootnoteText@ @footnote 1@ J. Viernow, J.-L. Lin, D.Y. Petrovykh, F.M. Leibsle, F.K. Men, F.J. Himpsel, Appl. Phys. Lett. 72, 948 (1998); J. Viernow, D.Y. Petrovykh, F.K. Men, A. Kirakosian, J.-L. Lin, and F.J. Himpsel, Appl. Phys. Lett. 74, 2125 (1999); D.Y. Petrovykh, J. Viernow, J.-L. Lin, F.M. Leibsle, F.K. Men, A. Kirakosian, F.J. Himpsel, J. Vac. Sci. Technol. A17, July/August (1999). @footnote 2@ Adam Li, Feng Liu, D.Y. Petrovykh, J.-L. Lin, J. Viernow, F.J. Himpsel, M.G. Lagally (to be published).

Topical Conference on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics
Room 6C - Session NT+NS+EM+MS-WeA
Nanotubes: Growth, Characterization and Properties I

Moderator: S.B. Sinnott, University of Kentucky

2:00pm **NT+NS+EM+MS-WeA1 Making and Modifying Carbon Nanotubes**, ***R.E. Smalley,*** Rice University **INVITED**

The last year has produced exciting developments in our ability to produce and modify single wall carbon nanotubes (SWNT). New experiments have shown the feasibility of producing nanotubes in an efficient gas-phase process, sometimes having diameters down to approximately 0.6 nm. These methods involve chemical vapor deposition in high-pressure carbon monoxide. We are now pursuing this growth technique as a potentially viable means for cost-effective production of large amounts of SWNT. Development of new methods for purification and characterization of nanotubes has given new insight into their growth mechanisms. I will present new data on the morphology and length distributions of SWNT grown by traditional laser-oven methods, and outline new results on the behavior and characteristics of tube samples. Perhaps the most remarkable developments have been in the chemistry of SWNT as a new molecular species. Several groups have discovered means of covalent attachment of other chemical species to the tube ends and sidewalls. This derivatization significantly modifies the properties of SWNTs, permits the first true solutions of tube segments, and opens the door to a remarkable new realm of chemistry, materials science, and electronics.

2:40pm **NT+NS+EM+MS-WeA3 Roles of Fe, Co, and Ni in the Formation of Single-Walled Carbon Nanotubes and Encapsulated Nanoparticles**, ***J. Jiao,*** Portland State University

The preparation and structural properties of carbon nanoclusters synthesized by having the transition metals Fe, Co, and Ni react with carbon in three different methods were investigated comparatively with the focus on single-walled nanotubes and encapsulated nanoparticles. The carbon nanoclusters were synthesized first by the high temperature (~3000°C) and high carbon-content process of the conventional arc discharge, secondly by the high temperature but low carbon-content process of the modified arc-discharge, and finally by the relatively low temperature (~500°C) process of catalytic decomposition of carbon monoxide (CO). The samples were characterized with respect to morphology, internal structure, and related properties. The carbon nanoclusters prepared by three different methods appear quite different on the surface, but have features in common that this report emphasizes. The same element can apparently serve different functions, serving as catalyst under one set of condition, and being encapsulated into the growing cages in a different environment. The elements of the iron group (Fe, Co, and Ni) were known as catalysts for growing the single-walled nanotubes and strings of spherical particles in conventional arc discharge, but could be encapsulated into the graphitic particles in the modified arc discharge and the CO disproportion that this study demonstrates. It was found that variation of the metal-to-carbon ratio is required to make these elements assume the double roles of either catalyst or encapsulant. In this report, an assembly of growth phenomena of carbon nanoclusters indicating the roles of the Fe, Co, and Ni will be presented. The growth mechanisms of these structural phenomena in relation to the preparation conditions in particular to the ratio of carbon content in the reaction chamber during the preparation are discussed.

3:00pm **NT+NS+EM+MS-WeA4 Plume Diagnostics During Carbon Nanotube Production by Laser Ablation**, ***S. Arepalli,*** G. B. Tech./Lockheed Martin; *C.D. Scott,* NASA/Johnson Space Center

We report recent results of our plume diagnostics during carbon nanotube production by double pulse laser oven method. The evolution characteristics of different species in the plume from different regions of the laser ablated plume will be presented. Transient emission data is compared with plume images to formulate dynamics of plume expansion. Vibrational and rotational temperatures of C@sub 2@ and C@sub 3@ are estimated by comparison with computations. Excitation spectra of LIF are used to deduce ground state temperatures and populations.

3:20pm **NT+NS+EM+MS-WeA5 Synthesis and Integration of Carbon Nanotubes**, ***H. Dai,*** Stanford University **INVITED**

This talk focuses on controlled growth and properties of multi-walled and single-walled carbon nanotubes on catalytically patterned substrates. It will be shown that new possibilities are opened up in nanotube science and applications by synthesizing nanotubes at desired locations and orientations in ordered fashions. A recently developed chemical vapor deposition method for high quality single-walled nanotubes is combined with microfabrication methods to reliably integrate single-walled nanotubes into various electrical architectures. The transport properties of individual single-walled nanotubes will be presented. Functional nanotube electrical devices with advanced performances will be shown. Issues in further control of nanotube growth will be addressed.

4:00pm **NT+NS+EM+MS-WeA7 Growth of Vertically Aligned Carbon Nanotubes on Transition-metal Catalyzed Plain Silicon Substrates using Thermal Chemical Vapor Deposition**, ***Y.H. Lee,*** *Y.C. Choi,* Jeonbuk National University, Korea; *C.J. Lee,* Kunsan National University, Korea; *Y.B. Han,* Jeonbuk National University, Korea

Vertically aligned carbon nanotubes have been grown on a large area of transition-metal coated plain silicon substrates by thermal chemical vapor deposition method. We find that vertically aligned growth is critically dependent on the domain density in the transition metal cluster. Steric hindrance between nanotubes at an initial stage of the growth forces nanotubes to align vertically. Nanotubes are then further grown by the catalyst-cap growth mechanism. We also show emission patterns from aligned nanotubes. Our current approach of simple integration of stable field-emission displays on a large area puts a step forward to future display applications.

4:20pm **NT+NS+EM+MS-WeA8 Carbon Nanotube Tips: Structures and Properties**, ***J. Han,*** *L. Yang, R.L. Jaffe,* NASA

A variety of structures and properties of carbon nanotube tips present challenges in understanding of electron tunneling and field emission of carbon nanotube materials. Topologically, a nanotube tip can be formed by joining a tube bulk and a cone or a half the fullerene. Different configurations can be resulted from arrangement of topological defects. Energetically favorable configurations are identified and classified using functional theory and molecular mechanics calculations. They are further used for electronic structure calculations based on tight-binding approaches. The location and intensity of localizes states at tips are studied as functions of the size and configurations of tips. The differences in localized stated between one and four-orbital calculations are also compared. Experimental results of carbon nanotube field emission properties are related to the calculations of the localized stated of nanotube tips.

4:40pm **NT+NS+EM+MS-WeA9 Electrochemical Deposition of Carbon Nanofilaments**, *E. Anoshkina,* ***D. Zhou,*** *L. Chow, V. Desai,* University of Central Florida

Carbon nanofilaments are conventionally made from thermal catalytic chemical vapor deposition with carbonaceous gases as growth precursors. Based on their unique mechanical, thermal, and electrical properties, many applications of carbon nanofilaments have been realized in advanced technologies. We report here on a new method to prepare carbon nanofilaments, in which the nanofilaments have been made from organic solvents such as methanol through an electrochemical deposition process. Silicon wafers coated with Fe or Ni nanoparticles were employed as the electrodes, and the depositions were carried out at room temperature. It has been found that electrical field between the electrodes, conductivity of the solvent, and size of the catalysts play important roles in control of morphologies of the carbonaceous deposits. Furthermore, based on characterization of the nanofilaments using scanning electron microscopy, transmission electron microscopy, and energy dispersive x-ray spectroscopy, the formation and growth mechanism of carbon nanofilaments from the electrochemical deposition has been discussed.

5:00pm **NT+NS+EM+MS-WeA10 A Study on the Growth of Carbon Nanotubes with Respect to Process Conditions**, *J.N. Srivastava, K.K. Awasthi,* ***C.D. Dwivedi,*** *G.N. Mathur,* Defence Materials & Stores Research & Development Establishment, India

Carbon nanotubes have been produced by graphite evaporation method in macroscopic quantities with reproducible results at different conditions. A study on the growth of CNT against the variation in Helium / Argon / Nitrogen pressure has been done and some interesting results are found with respect to geometry, density and alignment of the tubes. Total yield of

the material is also found to be having correlation with the pressure and current. Material produced in different conditions has been characterized by XRD, SEM, TEM, TGA and FTIR techniques.

Surface Science Division
Room 604 - Session SS3+NS-WeA

Islands, Clusters, and Steps

Moderator: J.C. Hamilton, Sandia National Laboratories

2:20pm **SS3+NS-WeA2 The Phase Diagram of a Self-Organizing Nano-Array**, ***K. Pohl***, *J. de la Figuera, M.C. Bartelt, N.C. Bartelt,* Sandia National Laboratories*; J. Hrbek,* Brookhaven National Laboratory*; R.Q. Hwang,* Sandia National Laboratories

Recent experiments show that in a submonolayer silver film on Ru(0001), a perfectly ordered array of nanometer-sized vacancy islands forms upon exposure to sulfur. By measuring the thermal vibrations of this equilibrium structure the forces responsible for the observed self-organization were identified and the elastic constants of the lattice derived.@footnote 1@ In order to develop a better understanding of the formation and ordering processes of this structure, we have explored the complete phase diagram of the vacancy island lattice. Via scanning tunneling microscopy we follow in real time the assembly of the hole lattice at different temperatures and S-Ag coverages. We find the hole lattice to be very robust against annealing cycles to 500 K. The final periodicity of the vacancy island lattice seems to be independent of the periodicity of the initial dislocation network in the strained silver film. This network only determines the initial etching sites for the S adatoms. The periodicity of the dislocation network in the clean Ag film depends on the Ag coverage. Beyond a threshold S-coverage, the array undergoes a phase transition to a periodic array of stripes. We will present a detailed study of the stability of these various novel equilibrium phases and identify the driving forces behind their formation. This work is supported by the Office of Basic Energy Sciences Division of Materials Sciences of the U.S. DOE (DE-AC04-94AL85000). @FootnoteText@ @footnote 1@K. Pohl et al., Nature 397, 238 (1999)

2:40pm **SS3+NS-WeA3 Tunneling on Ag and Au: Surface State Spectroscopy and Magic Molecular Clusters**, ***R. Berndt***, RWTH Aachen, Germany **INVITED**

We use low-temperature scanning tunneling microscopy (STM) to investigate geometric and electronic properties of nanoscale structures. In this presentation, we discuss various aspects of the Ag(111) surface state such as surface state confinement to nanometer-sized islands, its interaction with isolated magnetic impurity atoms, and the first study of lifetimes effects on Shockley surface state electrons using low-temperature STM spectroscopy. Moreover, we report on observations of two-dimensional supramolecular clusters and chains which self-assemble upon deposition of 1-nitronaphthalene (NN) onto Au(111). NN molecules become 2D-chiral upon adsorption. Their handedness is determined from from high-resolution STM images and local density calculations. Modeling shows that hydrogen bonds cause the observed self-assembly. Clusters and chains mutually interact via electrostatic repulsion.

3:20pm **SS3+NS-WeA5 Step Energetics of Pb(111) Vicinal Surfaces from Facet Shape**, ***H.P. Bonzel***, *K. Arenhold, A. Emundts, S. Surnev,* Forschungszentrum Jülich, Germany*; P. Wynblatt,* Carnegie Mellon University

The formation energies of steps and kinks, the step stiffness and the step interaction energy of B-steps vicinal to (111) have been derived quantitatively from the equilibrium shape of small three-dimensional Pb crystallites supported on a Ru(001) surface. The crystallites were imaged by scanning tunneling microscopy and show (111) and (100) facets.@footnote 1@,@footnote 2@ The boundary of these facets is well defined in the STM images and was used to determine also the azimuthal dependence of the step free energy for vicinal (111) surfaces by employing an "inverse" Wulff construction. Taking the accepted value for the surface free energy of Pb, absolute step energetic quantities can be quoted for both A- and B-steps. The step stiffness is derived from the step curvature and the step energy. The entropic step interaction energy of B-steps at 440 K is calculated from the step stiffness. Furthermore, by taking into account the curved portion of the vicinal (111) surface normal to the direction of B-steps, which shows a Prokovsky-Talapov behavior,@footnote 2@ the total step interaction energy of B-steps is also obtained. The entropic and total step interaction energies of B-steps at 440 K are thus 2.3 meV/Å@super2@ and 7.9 meV/Å@super2@, respectively.@footnote 3@ The difference is largely attributed to the elastic dipole-dipole interaction. Calculations of the step and elastic step interaction energies using the embedded atom potential of Pb@footnote 4@ are currently underway and will be compared with the experimental data. @FootnoteText@ @footnote 1@ S. Surnev et al., J. Vac. Sci. Technol. A 16(1998)1059. @footnote 2@ K. Arenhold et al., Surf. Sci. 417(1998)L1160. @footnote 3@ K. Arenhold et al., Surf. Sci. 424(1999)271. @footnote 4@ H.S. Lim, C.K. Ong, F. Ercolessi, Surf. Sci. 269/270(1992)1109.

3:40pm **SS3+NS-WeA6 Control of Monolayer Island Vacancies on Pt(111) and their Impact on Surface Chemistry**, ***K. Nafisi***, *J. Samu, J.C. Hemminger,* University of California, Irvine

Michely and Comsa@footnote 1@ have demonstrated that argon ion sputtering Pt(111) at elevated temperature will create ordered monolayer deep island vacancies. We show, by varying the surface temperature parameter, that it is possible to control the size of these vacancies over the range of 30Å to 400Å. We have used a variable temperature, scanning tunneling microscope (STM) to quantify the formation of the island vacancies. We have also used the STM to investigate the dehydrogenation of a series of mono-olefins to form carbon particles at 700 K. The carbon particles were formed both on a clean, annealed, and on sputtered Pt(111) surfaces. The carbon particles are randomly distributed over the surface, and show no preference for formation at particular surface features such as step edges. Also, the formation of the carbon particles is not influenced by large monolayer island vacancies. However, on a surface, where smaller island vacancies have been formed, the carbon particles show a preference of forming on the terraces and not inside of the island vacancies. The difference in behavior between large vacancy islands and small vacancy islands (d @<=@ 40Å) can be explained if molecular diffusion across steps is slow and dehydrogenation products initially decorate the walls (steps) of the vacancy islands. We have also studied the impact of sputtering the sample prior to olefin adsorption with the incident ion beam at an angle away from the surface normal. The carbon particles formed on such surfaces are highly spatially aligned. @super *@This work was supported by the US Department of Energy, Office of Basic Energy Sciences. @FootnoteText@ @footnote 1@ T. Michely and G. Comsa, Nucl. Instr. and Meth., B82, 207 (1993).

4:00pm **SS3+NS-WeA7 Coalescence Dynamics of Small Pt Clusters on Pt(111) Surfaces: A Molecular Dynamics Study**, ***V. Chirita***, *E.P. Münger, L. Hultman,* Linköping University, Sweden*; J.E. Greene,* University of Illinois, Champaign-Urbana

The diffusion and coalescence of small clusters are fundamental intralayer mass transport processes, playing a crucial role during the early stages of thin film deposition and crystal growth. We use embedded-atom method molecular dynamics simulations to follow the kinetics characterizing these processes for compact, 2D Pt@sub 5@ and Pt@sub 6@ clusters on Pt(111), at 1000 K. Investigations are carried out for configurations consisting of clusters initially separated by a distance equal to that between second neighbors, in statistically independent runs of 10 ns each. Prior to coalescence, we observe that the intercluster separation distance is reduced via two pathways: net cluster diffusion, involving mechanisms which preserve cluster shape, and repeated cluster reshaping. Cluster diffusion occurs primarily via concerted gliding and reptation, a recently proposed diffusion mechanism for 2D clusters on (111) metallic surfaces. Cluster reshaping involves edge-diffusion and/or concerted dimer/trimer gliding. Our simulations reveal that cluster coalescence is achieved via complex dynamics. Clusters preserving their initial compact shape can coalesce via concerted gliding and form clusters with a high number of intracluster bonds. These larger clusters maximize the number of intracluster bonds in relatively short times, primarily via edge-diffusion. We observe for the first time, that during the fusion process, cluster-cluster interactions can induce cluster translations via sequential atom motion, through fcc/hcp bridge sites, within clusters. For clusters that reshape prior to coalescence, we observe that cluster-cluster interactions induce the transfer of single atoms, from either cluster, to sites neighboring both clusters, and thus create a "bond" between clusters. Once formed, we did not observe dissociation. In this case, the newly formed clusters have elongated shapes with narrow middle sections (1 to 2 atoms thick) and, as a result, the transition toward compactness is achieved over considerably longer times. Moreover, these clusters exhibit a variety of reconfiguration and migration events. Edge-diffusion, reptation and dislocation propagation are the competing diffusion mechanisms observed for clusters in this range.

4:40pm **SS3+NS-WeA9 Spontaneous Island Formation on the GaAs(001) 2x4 Reconstructed Surface**, ***P.M. Thibado***, *V.P. LaBella, M. Anser, Z. Ding, D.W. Bullock,* University of Arkansas

Given the growing use of III-V semiconductor materials in wireless and high speed communication devices the preparation of atomically flat single crystal GaAs(001) surfaces was examined, since these devices are primarily fabricated using epitaxial methods . To achieve this, a state of the art molecular beam epitaxy (MBE) system with a novel temperature measurement system accurate to within ±2 @super o@C, has been combined, in situ, with a scanning tunneling microscope (STM). Surprisingly, when the GaAs(001) 2x4 reconstructed surface is annealed above a critical temperature (570 @super o@C), under a constant As@sub 4@ flux, it spontaneously forms one monolayer high islands covering one half of the otherwise flat terraces. This process is reversible and when fit to a free energy model yields information about the surface bonding energies. This work was funded in part by the National Science Foundation (DMR-9733994) and the Office of Naval Research (N00014-97-1-1058).

5:00pm **SS3+NS-WeA10 TiN(001) Epitaxy: An in-situ Temperature-Dependent STM and Level-Set Modeling Study**, *S. Kodambaka,* ***P. Desjardins***, *A. Vailionis, I. Petrov, J.E. Greene,* University of Illinois, Urbana*; D. Chopp,* Northwestern University

We have used in-situ temperature-dependent STM measurements during deposition and post-annealing combined with modeling to provide atomic-scale insights into surface morphological evolution during TiN growth. Epitaxial TiN(001) layers were grown by reactive evaporation onto MgO(001) at 700-950 @super o@C. Partial TiN monolayers (0.1-0.4 ML) were then deposited and in-situ high-temperature STM used to follow the coarsening and decay kinetics of single and multiple islands (Ostwald ripening) on flat terraces and in single-atom deep vacancy terraces. From these results, combined with finite-element solutions of the Gibbs-Thompson and diffusion equations, we obtain the activation energy for surface diffusion, the Ehrlich barrier energy, and the island line tension. We have also derived and implemented a level-set method for simulating the dynamics of island decay on time scales not accessible to experiment. Level-set methods are numerical techniques for computing the position of propagating fronts that can easily handle topographical changes as well as singularities including corner and cusp development. Our model includes geometry-dependent surface and edge diffusion, step-edge dynamics, and attachment/detachment rates. We compare our numerical results to in-situ STM time-sequence experiments under the same conditions. The results of the level-set calculations serve as a basis for a robust quantitative and predictive model for both microstructural and surface morphological evolution as a function of deposition conditions during polycrystalline TiN growth.

Nanometer-scale Science and Technology Division
Room 4C - Session NS-WeP

Poster Session

NS-WeP1 Tip Passive Chemical Modification and Its Effects on Tribological Measurements, ***X.D. Xiao***, *L.M. Qian,* The Hong Kong University of Sci. & Tech., China

In this talk, we present our experimental results on the passive chemical modification process of the silicon nitride AFM tip by OTE/Mica, OTE/SiO@sub 2@, and SiO@sub 2@. The modified tips have different friction and adhesion properties against mica reference samples as compared to their pristine conditions. The resultant tip modification not only depends on the OTE SAM but also on the substrates the OTE SAM is prepared on. In the case of OTE/Mica, the friction of the modified tip against mica reference is much reduced; in the case of OTE/SiO@sub 2@, the friction of the modified tip against mica reference is much increased. It is surprising that bare SiO@sub 2@ can also chemical modify the Si@sub 3@N@sub 4@ tip to increase the friction against mica reference. In the case of OTE modification, it was found that the tips could be cleaned by repetitive friction scans on mica. However, tip modified by SiO@sub 2@ cannot be mechanical cleaned. Moreover, it was also found that humidity and load could also affect the tip chemical modification. Our results here is important for interpreting tribological data since the actual contact chemistry was often over-looked in the AFM experiments in the past.

NS-WeP2 Velocity Dependent Friction, ***J.A. Heimberg***, *K.J. Wahl, I.L. Singer,* Naval Research Laboratory*; A. Erdemir, G. Fenske,* Argonne National Laboratory

Low friction, low wear diamond-like carbon (DLC)@footnote 1@ films have been studied under dry N@sub 2@ and dry air using a reciprocating tribometer. It was found that as the velocity decreased from mm's/sec to 10's μm/sec the friction coefficient dropped over an order of magnitude. The friction behavior was dependent on environment and counterface material. Tracks and balls have been analyzed for wear using optical and Raman microscopy. Conditions leading to the lowest friction will be discussed. The friction behavior can be quantitatively described in terms of gas adsorption models. @FootnoteText@ @footnote 1@ Work partially supported by the U.S. Department of Energy under Contract W-31-109-Eng-38. .

NS-WeP3 Gold Nano-wire Fabrication on Si(111) Using Piezoresistive Cantilevers, ***T. Uchihashi***, *U. Ramsperger, H. Nejoh,* National Research Institute for Metals, Japan

Recent development of STM-based technology offers us unique opportunities to fabricate nano-scale structure in various ways in ultra-high vacuum (UHV). Although it is getting more and more established, measurement of electron conduction through nanostructures made in UHV has not been realized yet, except for scanning tunneling spectroscopy. Considering that there is a great demand for downsizing electronic circuit to nano-scale level, and that clean UHV condition is desirable to avoid surface contamination, such a measurement is highly demanded. Here, we present a novel but simple way of fabricating nano-scale metal wire on a clean substrate in UHV, which will enable us to realize such a measurement. As a gold-coated atomic force microscope (AFM) cantilever is brought into contact with a Si(111) sample surface, gold was transferred onto the sample surface, forming wires while the cantilever was moved laterally on the surface. Piezoresistive cantilevers (Piezolever,@footnote 1@ spring constant 2 - 10 N/m) were first coated with gold by thermal evaporation to a thickness of 50 to 60 nm. To fabricate gold wires on Si(111) surface, a gold-coated cantilever was brought into contact with sample surface and was moved laterally in a speed of 4 -32 nm/s. After this procedure, clear protruded line patterns were observed using STM. The minimum width of the lines was around 23 nm. In non-contact AFM mode, however, we found unusual line contrast change, according to the polarity of tip bias voltage. The probable reason for the line contrast change is charge transfer between silicon surface and gold. We also succeeded in connecting gold nano-wires to silver electrode pads, which was made by thermal evaporation in situ. The electrode pattern was defined by a through-hole mask, which was made of a titanium foil cut by focused ion beam. This demonstrates the possibility of measuring the properties of electron conduction through nanostructures made in UHV. @FootnoteText@ @footnote 1@ Courtesy of Park Scientific Instruments

NS-WeP4 Dual-Wavelength Scanning Near-Field Optical Microscopy, ***P.R. LeBlanc***, *M. Gu, P. Grutter,* McGill University, Canada*; D. Gray,* PAPRICAN, Canada

We have developed a dual-wavelength Scanning Near-Field Optical Microscope to investigate biological samples in air. Using a helium-cadmium laser, we couple 442 nm and 325 nm light into a tapered optical fiber. Light transmitted through the sample is detected in a confocal arrangement. A dichroic mirror separates the two optical channels which are then detected by photomultipliers. The fiber tip is shaped, by immersion into a buffered hydrofluoric acid solution, to an aperture of less than 100nm and then coated with aluminum, defining a true sub-wavelength light source. Once coated, the tip is glued onto one of the tines of a quartz tuning fork which is then oscillated either parallel or perpendicular to the sample surface a few nanometers away. We have found that the latter method (gently tapping the surface) yields a resolution of greater than 20 nm topographical and 50 nm optical. An optical and topographical standard was created by lift-off of a 100 nm aluminum film evaporated on a close-packed monolayer of 500 nm diameter polystyrene spheres. Our initial focus for this instrument has been centered on the investigation of the lignin distribution in Black Spruce fibers. Lignin, a cross-linked phenolic polymer, is of paramount importance in the pulp and paper-making processes. It is a primary component of the wood cell wall and absorbs preferentially in the ultraviolet (it is the only component of the cell to do so). The dual-wavelength capability of our instrument permits the discrimination between chemical species density and topographical variations of the sample as well as near-field optical artifacts.

NS-WeP5 Influence of Secondary Tip Shape and Imaging Mode on Illumination Mode NSOM Images, ***S.J. Stranick***, *C.E. Jordan, G.W. Bryant, R.R. Cavanagh, L.J. Richter,* National Institute of Standards and Technology

We report illumination-mode near-field optical microscopy images of individual 80-115 nm diameter Au particles with metal-coated fiber probes. It is found that the images are strongly influenced by the thickness of the metal coating. Theoretical models are presented which are in good agreement with the images. Wide probes with thick coatings (~lambda/2) produce images consisting of three extrema, due to a resonance-like polarization of the probe end. Narrow probes with thinner coatings produce wavy images, due to interference between the direct radiation from the tip and propagating tip fields scattered by the particles. Additionally, we have demonstrated a method for acquiring images that allows for the construction of three different imaging modes from one data set: constant-gap, constant-height, and constant-intensity. The method is based on the acquisition of topographic and optical data in a three-dimensional rather than a two-dimensional scanning format with controlled scans along the dimension normal to the surface. In this way, we acquire the topographic features of the sample surface as well as its optical response at various heights. This allows for the construction of constant-height and constant-gap images from the same data set and provides a means of identifying and correcting features that are a result of topographically induced optical contrast. Comparison between images recorded in this format to images 'lift-off' corrected by a single or small number of retraction curves indicates significant artifacts can still be present in corrected images.

NS-WeP6 InGaAs Quantum Dots fabricated by Separated-Phase Enhanced Epitaxy with Droplets (SPEED), ***T. Mano***, *K. Watanabe, S. Tsukamoto, Y. Imanaka, T. Takamasu,* National Research Institute for Metals, Japan*; H. Fujioka,* University of Tokyo, Japan*; G. Kido,* National Research Institute for Metals, Japan*; M. Oshima,* University of Tokyo, Japan*; N. Koguchi,* National Research Institute for Metals, Japan

Highly uniform InGaAs quantum dots (QDs) were successfully grown by Separated-Phase Enhanced Epitaxy with Droplets (SPEED) method. The SPEED is a novel method for self-organizing growth with highly dense Ga droplets produced by Droplet Epitaxy.@footnote 1@ All samples were grown on GaAs (001) substrates by molecular beam epitaxy method. After the growth of a GaAs buffer layer, an As-stabilized c(4x4) surface was formed as an initial surfaces. On this surface, 1.75ML of Ga, 2.5ML of In, and 50ML of Ga were supplied at 200°C, in order to compensate the 1.75ML excess As on c(4x4), to form the InGa droplets, and to form the highly dense Ga droplets surrounding the InGa droplets, respectively. After the formation of these droplets, which were very uniform in size, As flux was supplied at 200°C for crystallization and the sample was annealed at 500°C. At that time, the highly dense Ga droplets prevented the 2-dimensinal growth of the InGaAs and the separated-phase effect of InGaAs-

GaAs was enhanced. Finally, a GaAs capping layer was grown. To confirm the effect of highly dense Ga, a reference sample was also fabricated with the same procedure except for the supply of 50ML Ga. In the case of the sample with the 50ML of Ga, not Stranski-Krastanov (S-K) mode but a flat surface is observed after the crystallization and annealing process. However, without 50ML of Ga, the S-K mode occurs. Although photoluminescence spectra of these samples are observed at same wavelength around 950 nm, the FWHM of the PL spectrum with 50ML Ga (22meV) is narrower than that of without 50ML Ga (100meV), and the intensity of PL spectrum with 50ML of Ga is thirty times stronger than that of without 50ML Ga. These results indicate that the uniform InGa droplets changed into the uniform InGaAs QDs embedded in GaAs. Therefore, the SPEED is very useful fabrication method for the high quality InGaAs QDs. @FootnoteText@ @footnote 1@ N. Koguchi and K. Ishige, Jpn. J. Appl. Phys. 32, 2057 (1993).

NS-WeP7 Diamond Growth from a Reconstructed Diamond(100) Monohydride in a Non-uniform Electric Field, ***J.K. Kang,*** Stanford University

We will present the effect of an electric field on the growth from a reconstructed diamond(100) monohydride with mechyl radical of CH3 with a growth species, which was examined at the ab initio density functional cluster calculation of the B3LYP theory. First of all, activation energies of various reaction steps involving in this growth under a non-uniform electric field, which is calculated using the electron orbital energies and vibration frequencies of these various reaction steps via the ab initio cluster calculation on cluster models, C9H14 and C38H40, will be compared to activation energies without an electric field. Finally, we will address that the non-uniform electric field can drastically change the surface reaction pathway by modifying the electronic structures and vibration frequencies, which corresponds to the modification of activation energies of various reaction steps involving in this growth.

NS-WeP8 Fabrication of a Nanosize Metal Aperture for NSOM Sensor using PR Removal and Sputtering Techniques, *M.Y. Jung, I.W. Lyo,* Yonsei University, Korea; ***S.S. Choi,*** Sun-Moon University, Korea

The scanning near-field optical microscopy(NSOM) can be used for imaging on a nanometer scale and identifying individual molecules with capability to surpass the resolution-limiting diffraction of conventional optical methods.@footnote 1@ In order to obtain better resolution limit, the diameter of the thin metal aperture has to be less than the optical wavelength. The fabricated nanosize Si tip using RIE have been thermally evaporated with a Au or Cr metal thin film. In order to have an aperture with diameter less than 100nm on top of the tip, several methods have been applied including sputtering and photoresist-stripping techniques.@footnote 2@ We have successfully fabricated the metal aperture with diameter less than ~0.3 nm on the silicon nitride tip. @FootnoteText@@footnote 1@ R.C. Davis, C.C. Williams and P. Neuzil, Appl. Phys. Lett. 66(1995) 2309. @footnote 2@M.Y. Jung, I.W. Lyo, S.S. Choi, MNE98, Sept.15-21, Leuven, Belgium. .

NS-WeP9 Non-destructive 1-D SCM Dopant Profiling Determination Method and Its Application to the 3-D Dopant Profiling, ***E.-S. Kang***, *J.-W. Kang, H.-J. Hwang,* Chung-Ang University, Korea

As the scaling of feature size in the GSI device technology is continuing, the device characterization and life cycle is greatly affected due to an unexpected doping profile which is caused by 3-dimensional effects in mask corners and edges. Therefore, the experimentally determined 3-D impurity doping profile is needed to estimate these 3-D effects precisely. In this work, we present a new 1-D doping profiling determination method, which extends to the quantitative 3-D dopant profiling extraction. This is the non-destructive technique and method, which is different from conventional AFM/SCM measurement/dopant extraction and we can measure directly at real MOSFET device having 3-D structure. Through SCM modeling, we found the depletion layer in silicon was of a form of spherical capacitor with SCM tip biased. 2-D FDM (Finite Differential Method) code with SOR (Successive Over Relaxation) solver was developed to model the measurements by a SCM of a semiconductor wafer that contains an ion-implanted impurity region. And we analyzed this capacitor theoretically and determined the depleted total volume charge (Q), capacitance (C) and the rate of capacitance change with bias (dC/dV). It is very important to observe the depleted carriers movement in the silicon layer by applying a bias to tip. So we calculated the depleted volume charge considering some factors such as tip size, oxide thickness and applied bias (dc + ac) which has effect on the potential and depletion charge. Finally, we developed 1-D inversion algorithm to convert SCM measurement output (dC/dV) into real dopant concentration, comparing SCM signal output with the calculated dC/dV through SCM modeling. We assume 1-D Pearson distribution function having several parameters as the initial profile. This profile extraction procedures consist of finding the profile that minimizes the least squares fit criterion between the calculated dC/dV and the measured dC/dV.

Topical Conference on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics

Room 4C - Session NT+NS+EM+MS-WeP

Poster Session

NT+NS+EM+MS-WeP1 Growth of Carbon Nanotubes at Low Temperature by Microwave Plasma-enhanced Chemical Vapor Deposition, ***Y.C. Choi,*** *D.J. Bae, Y.H. Lee, B.S. Lee,* Jeonbuk National University, Korea

We have grown carbon nanotubes at temperatures below 520 C by microwave plasma-enhanced chemical vapor deposition using methane and hydrogen gases. Carbon nanotubes were uniformly grown in large area of transition metal-coated Si substrates with high density. Each nanotube is terminated by transition metal cap, suggesting that the transition metals play an important role in the nanotube growth. Carbon nanotubes are curly in all cases, indicating the nanotubes to be defective due to very low growth temperature. Diameters and lengths of the nanotubes could be controlled by changing the ratio of methane to hydrogen and growth time. Raman spectum clearly shows the peak at 1592 cm-1 (G-band), indicating the formation of well graphitized carbon nanotubes.

NT+NS+EM+MS-WeP2 Nanoscale-controlled Handling of Carbon Nanotubes, ***O. Jaschinski***, *P. Bernier, L. Vaccarini, C. Goze,* Universite Montpellier II, France; *G. Duesberg,* Trinity College Dublin, Ireland; *C. Journet, S. Roth,* Max-Planck-Institut fuer Festkoerperforschung Stuttgart, Germany

Carbon nanotubes are the most promising materials for applications in nanoelectronics and nanomechanics. For the determination of the electrical and mechanical properties of nanotubes and for the production of nanotube devices one needs the ability to handle nanoscale materials in a controlled way . We demonstrate how atomic force microscopy (AFM) can be used as a tool for manipulating and investigating carbon nanotubes. For an optimal use of AFM it is necessary to control the substrate-nanotube interaction. We present results of measurements of the mechanical properties of nanotubes obtained with various kinds of substrates. We show how the combination of lithography, manipulation by AFM and control of the adsorption process of nanotubes allow to prepare well defined sample configurations for very sophisticated measurements of the electrical and mechanical properties of carbon nanotubes. Based on these methods, techniques for the production of nanotube devices can be developed. This work was supported by European TMR contract NAMITECH ERBFMRX-CT96-0067 (DG12-MIHT)

NT+NS+EM+MS-WeP3 Aligned Carbon Nanotubes with Controlled Diameters Using Anodic Alumina Template, ***S.-H. Tsai***, *H.C. Shih,* National Tsing Hua University, R.O.C.

The microwave plasma enhanced chemical vapor deposition (MPECVD) system had been successfully fabricated the well-controlled diameters of aligned carbon nanotubes on the anodic alumina template with a mixture of methane and hydrogen. Prier to test, the anodic alumina with pore arrays in various diameters were prepared by anodizing aluminum using oxalic, sulfuric, and phosphoric acid solutions. By adjusting the pore size of the anodic alumina, various carbon nanotube diameters can be obtained in a range of 30 to 100 nm and were examined by scanning electron microscopy and transmission electron microscopy.

NT+NS+EM+MS-WeP4 The Selective Growth of Aligned Carbon Nanotubes by PECVD Using Nickel Catalyst, ***H. Jeon***, *K. Ryu, M. Kang,* Hanyang University, Korea

Carbon nanotubes have been studied extensively because of their own unique physical properties and also of their application potential for field emitters. One of the interesting applications is reported for display application, but neither industrial fabrication technology nor performance has been reported for practical display application. Here we tried to grow aligned carbon nanotubes selectively by plasma enhanced chemical vapor deposition (PECVD) method using nickel catalyst@footnote 1@ at temperatures below 600°C. These conditions for low temperature growths are suitable for field emission display which requires carbon nanotube

emitters grown perpendicular to the Si substrate. In our experiment, a thin film of nickel(10-100nm) was deposited through a pattern mask on a Si substrate in UHV e-beam evaporator and was agglomerated by in-situ annealing for thirty minutes at 700°C. The use of a patterned catalyst enhanced the formation of selectively aligned nanotubes at low temperatures. After this process, Ni particles deposited on Si substrate were examined by AFM and SEM. Carbon nanotubes were selectively grown on Ni particle by PECVD with using the mixture of CH@sub 4@ and NH@sub 3@ at 600°C. In this process, CH@sub 4@ was used as the carbon source and NH@sub 3@ was used as a catalyst and dilution gas. During the process, many carboneous impurities can be produced and tried to eliminated by introducing H@sub 2@ plasmas. We examined the physical properties of carbon nanotubes by SEM, XRD and Raman spectroscopy. And we investigated the formation temperature of carbon nanotubes on silicon substrate and controlled the selective growth of aligned nanotubes. @FootnoteText@ @footnote 1@ Masako Yudasaka, et al.,Appl. Phys. Lett. 70(14), 7 April 1997.

Magnetic Interfaces and Nanostructures Technical Group
Room 618/619 - Session MI+NS-ThM

Patterned or Self-Assembled Magnetic Nanostructures

Moderator: Z.Q. Qiu, University of California, Berkeley

8:20am **MI+NS-ThM1 1-D Propagation of a Magnetic Domain Wall in Submicron Magnetic Wire**, ***T. Ono***, *H. Miyajima,* Keio University, Japan; *K. Shigeto, K. Mibu, N. Hosoito, T. Shinjo,* Kyoto University, Japan **INVITED**

A novel method to detect single domain wall motion in a submicron magnetic wire by utilizing the giant magnetoresistance (GMR) effect is presented.@footnote 1@ Recent developments of nanolithography techniques make it possible to prepare submicron dots or wires with well-defined shape, leading to the current attention on the quantum phenomena in mesoscopic magnetic materials, such as macroscopic quantum tunneling and macroscopic quantum coherence. However, the direct magnetization measurements of mesoscopic magnetic materials are practically difficult because of their small volume, and have been performed using samples consisting of a huge number of presumably identical particles. As a result, the essential magnetic properties of a single particle or wire were masked by the inevitable distribution of size or shape. Up to now, quantitative measurements on dynamical properties of a domain wall in a submicron magnetic wire, such as velocity estimation were almost impossible. The method described in this paper has a great advantage to detect a single magnetic domain wall motion, since the GMR change is directly proportional to the magnitude of the switching layer magnetization in a magnetic wire. It should be noticed that the domain wall position can be determined by this method as a function of time, and, thus, we can measure the velocity of a single domain. The wall velocity linearly depends on the applied magnetic field H and is described as v = μ(H - H@sub 0@), where v is the wall velocity, μ so-called wall mobility. In case of NiFe wire 40 nm in thickness and 500 nm in width, it was obtained that μ = 2.6 (m/sOe), and H@sub 0@ = 38 (Oe) at 100 K. @FootnoteText@ @footnote 1@ T. Ono, H. Miyajima, K. Shigeto, K. Mibu, N. Hosoito and T. Shinjo, Science, 284 (1999) 468-470.

9:00am **MI+NS-ThM3 Magnetism of Interconnected Co Nanodots Grown on the N-modified Cu(001) Surface**, ***K.D. Lee***, *T. Iimori, F. Komori,* University of Tokyo, Japan

Square arrays of ultrathin Co nano-size dots interconnected by 1 monolayer-height Co nanostripes are grown on the N-modifed Cu(001)c(2x2) substrate. Scanning tunneling microscopy shows the Co atoms are nucleated at the naked Cu(001) substrate exposed between ordered arrays of c(2x2) square patches forming such a novel Co nanostructure. The sizes of Co dots and interconnecting nanostripes are controlled by the amount of Co deposition at room temperature. Magnetic properties of these nanostructures have been investigated by using magento-optical Kerr effect between 100 K and 450 K. Analysis of hysteresis loops as a funtion of temperature as well as thickness reveals that these Co dot arrays have remarkably different magnetic properties from ultrathin fcc Co films grown on clean Cu(001) surface with the same average thickness, such as two-step increase of the saturation magnetization and coercivity with decreasing temperature. We attribute these novel magnetic properties to the magnetic interaction among Co dots mediated by the interconnecting Co stripes.

9:20am **MI+NS-ThM4 Periodic Magnetic Microstructures using Glancing Angle Deposition**, ***B. Dick***[1], *M.J. Brett, M. Malac, R.F. Egerton,* University of Alberta, Canada

Arrays of magnetic pillars have been proposed as a potential high-density data storage medium.@footnote 1@ The advanced deposition technique known as GLancing Angle Deposition (GLAD)@footnote 2@ has been used to fabricate Ni and Co posts. Because of the nature of initial film nucleation, these posts were distributed randomly on the substrate surface with a large-scale periodicity of around 350nm and individual post diameters of 100 to 150nm. We have grown arrays of posts by suppressing the randomness inherent within the initial nucletion stage of film growth. Shadowing sites were fabricated by pre-patterning a thin Cr or Ti layer on silicon substrates into a square array using electron beam lithography. These sites shadow regions of the substrate from incident flux during film deposition and act as preferred nucleation sites for the Ni and Co pillars. Using this process, we have obtained a regular post period of 500nm, with post diameters and heights of 300nm and 375nm respectively. This presentation will describe the GLAD deposition process, report on the film's periodic structure, and characterise the film's domain structure (MFM) and hysteresis response curve. Further development on decreasing the period between individual posts is continuing, and we exptect that 200nm spacing should be attainable using this simple, single-step evaporation process. @FootnoteText@ @footnote 1@S.Y. Chou. Proceedings of the IEEE. 85(4), 1997. @footnote 2@K. Robbie, J.C. Sit, M.J. Brett. J. Vac. Sci. Technol. B. 16(3), 1998.

9:40am **MI+NS-ThM5 Magnetic Quantum Cellular Automata**, ***R.P. Cowburn***, University of Cambridge, UK, United Kingdom; *D.K. Koltsov, A.O. Adeyeye, M.E. Welland,* University of Cambridge, UK **INVITED**

Nanometre scale magnetic particles (nanomagnets) are promising candidates for implementing Magnetic Quantum Cellular Automata (MQCA) architectures. In order to use nanomagnets in this way their magnetic properties must be fully understood. In particular, the conditions required to obtain a single domain state (and hence the ability to signal a 1 or a 0) must be established. Furthermore, in order to achieve room temperature operation of MQCA, magnetostatic coupling between nanomagnets must be understood and controlled. We have performed a detailed experimental and theoretical investigation into these aspects of nanomagnetism. We have used high resolution electron beam lithography to fabricate nanomagnets in the size range 40-500nm with elliptical or circular geometries. We find that the shape anisotropy introduced by the elliptical form greatly stabilises the single domain state; in the absence of any ellipticity, all of the nanomagnets greater than approximately 100nm in diameter collapse into a flux closing vortex state. We have then fabricated chains of sub-100nm nanomagnets with gaps as small as 15nm between neighbouring edges. We find experimental evidence for strong magnetostatic coupling. We have thus achieved the conditions necessary for a MQCA implementation, i.e. a well defined digital state even at room temperature which can be switched by interactions from neighbouring cells. We have used the finding described above to make a working room temperature MQCA gate. CMOS electronic signals are interfaced directly to the magnetic system by passing a small current through a gold track underneath part of the gate; outputs are currently read by focusing a laser beam onto a magnetic test point and using the magneto-optic Kerr effect to monitor its magnetic state. The gate achieves an overall power gain (and hence the ability to work at room temperature and to fan out) by an applied oscillating magnetic field.

10:20am **MI+NS-ThM7 Growth, Magnetization, and Magnetoresistance of Self-Assembled Lateral Multilayers**, *E.D. Tober,* Lawrence Berkeley National Laboratory; ***R.F. Marks***, *D.D. Chambliss, R.F.C. Farrow,* IBM Almaden Research Center

The angular dependent magnetoresistance, magnetization, and growth of epitaxial Fe@sub eta@Ag@sub 1 - eta@ self-assembled lateral multilayers@footnote 1@ (SALMs)have been examined via MOKE, 4-point resistance probes, STM, LEED, X-ray MCD, and TEM. SALMs consist of epitaxial thin film alloys of immiscible metals grown on Mo(110)/Al@sub 2@O@sub 3@(11-20) template layers and display a unique form of compositional ordering not observed in the bulk. These systems are observed to form a compositionally ordered alloy of alternating, contiguous stripes of Fe and Ag with the long axis of the stripe coinciding with the Mo[001] direction in the plane of the substrate. The average stripe periodicities are on the order of 1.8 to 2.3 nm along the Mo[-110] (perpendicular to the stripes) direction depending on film stoichiometry. These films are found to contain a high degree of magnetic anisotropy with the easy direction lying in-plane parallel to the Mo[001] direction. The low temperature anisotropic magnetoresistance (AMR) and low field magnetoresistance (MR) are examined as a function of field angle for two nearly orthogonal current directions. The SALM structures are observed to display a significant AMR (roughly 10% maximum for the entire structure). Furthermore, a pronounced MR is observed with a maximum @Delta@R/R of 0.88% (~29% in the active layer) at 2.7 K. @FootnoteText@ @footnote 1@ "Self-assembled lateral multilayers from thin film alloys of immiscible metals", E. D. Tober, R. Farrow, R. Marks, K. Kalki, G. Witte, and D. D. Chambliss, Phys. Rev. Lett. 81 N9, 1897.

10:40am **MI+NS-ThM8 Stripe Domains in Ultraflat Fe/Cu(001) Particles**, ***C. Stamm***, *A. Vaterlaus, U. Maier, D. Pescia,* ETH Zuerich, Switzerland

Atomically thin particles of Fe on Cu(001), grown at room temperature, are investigated using a Scanning Electron Microscope with Polarization Analysis (SEMPA): a Mott detector is used to analyze the perpendicular as well as one of the in-plane spin components of the secondary electrons.

[1] **Falicov Student Award Finalist**

The magnetic particles with thickness of a few atomic layers are produced by Molecular Beam Epitaxy through a mask placed in front of the Cu substrate. As in laterally extended thin films of Fe/Cu(001), particles whose lateral size exceed 1 μm contain stripe domains with magnetization perpendicular to the film plane. The width of the stripes is independent of the lateral size of the particles and their shape. Sizing down the Fe particle leads to a single-domain configuration. In contrast, in-plane magnetized ultrathin Co/Cu(001) particles are found in a single domain state, irrespective of their lateral size.@footnote 1@ @FootnoteText@ @footnote 1@C. Stamm, F. Marty, A. Vaterlaus, V. Weich, S. Egger, U. Maier, U. Ramsperger, H. Fuhrmann and D. Pescia, Science 282, 449 (1998).

11:00am **MI+NS-ThM9 Magnetic Properties of Iron Clusters Deposited on Graphite**, ***A. Rosén,*** *M. Andersson,* Göteborg University, Sweden*; M. Hansson,* Chalmers University of Technology, Sweden*; R. Wäppling, B. Kalska,* Uppsala University, Sweden*; N. Tarras-Wahlberg,* Göteborg University, Sweden*; C. Johansson,* Chalmers University of Technology, Sweden

Magnetic properties of iron clusters deposited on graphite Iron clusters with a wide size distribution were produced in a laser vaporisation source and deposited on a graphite substrate. The magnetic relaxation of the clusters was studied with Mössbauer spectroscopy. At 300 K the sample was dominated by fast superparamagnetic behaviour, whereas the relaxation slowed down at lower temperature and six-peak components, representative for static or near-static spinconfigurations, dominated the Mössbauer spectra at 5 K. This indicates that the sample consists of mono-domain particles having an average size between 5 and 10 nm. From the hysteresis loops we obtained that the saturation magnetization was in the range of bulk a -iron and that the coercivity and the remanence increase with decreasing temperature in the whole temperature range. This behaviour is typical for a system of mono-domain particles with a wide size distribution.

11:20am **MI+NS-ThM10 Magnetic Properties of Co and Fe Particles on Sapphire Single Crystal Surfaces**, ***T. Risse,*** *T. Hill, M. Mozaffari-Afshar, H.-J. Freund,* Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

We have used in situ Ferromagnetic Resonance (FMR) to investigate the magnetic properties of small Co and Fe particles deposited on sapphire single crystal surfaces. Co and Fe grow as 3-dimensional particles, as deduced from the angular dependence of the FMR spectra. This result was confirmed by STM studies on an Al@sub 2@O@sub 3@ model surface grown on top of a NiAl(110) single crystal. The FMR spectra of Co or Fe particles deposited at 298 K reveal a uniaxial out-of-plane magnetization with the magnetization lying in the surface plane. A comparison of the measured angular dependence of the resonance position with 2-dimensional films show that experimental results are consistent with a 3-dimensional growth of the particles determined by the STM measurements. A closer examination of the FMR spectra indicates that these small particles exhibit superparamagnetism. With increasing amount of deposited metal the anisotropy of the systems increases indicating a more ferromagnetic behavior of the system. Annealing the samples to elevated temperatures (900K) leads to structural changes of the particles namely an increase of the particle size as deduced from FMR and Auger spectroscopy. Whereas the qualitative behavior of the magnetic anisotropy for Co deposits remains unchanged, the behavior of the iron particles changes drastically. The particles do not show a uniaxial anisotropy of a single resonance line but a complex pattern of several resonance lines. A discussion of this aspects in terms of shape as well as magnetocrystalline anisotropy will be given. Temperature dependent measurements of the Fe particles reveal a reduced Curie temperature compared to the bulk. The strong changes of the line shape with increasing temperature will be discussed in terms of a thermal fluctuations of the magnetization.

11:40am **MI+NS-ThM11 Magnetic Behavior of Nanosize Cobalt Particles in (SiO@sub 2@, MgO, CoO) Matrix**, ***J.Y. Yi,*** *M.L. Rudee,* University of California at San Diego

Magnetic granular composite films composed of nanosize metal particles separated by a non-magnetic matrix, have interesting magnetic properties due to the finite size of the metal particles. Recently we found that ferromagnetic (FM) and antiferromagnetic (AFM) composite films such as Co-CoO films had much larger coercivity (~1 kOe at 300 K) than conventional granular Co-SiO@sub 2@ films (superparamagnetic at 300 K) in the same composition range. The increased coercivity was believed to be due to the exchange coupling between FM Co and AFM CoO, and the microstructure of the Co particles. These results indicated that the overall properties of the metal phase were affected by not only the intrinsic properties of them but also the characteristics of the matrix phase. To examine the matrix effects, Co-SiO@sub 2@, Co-MgO and Co-CoO granular composite films were prepared by co-sputtering from separate Co and each oxide target. Each film had 30~40 volume % of Co. The estimated Co particle size from x-ray peak broadening effect was about 7 nm. Magnetic hysteresis loops showed that the superparamagnetic behavior of Co at room temperature in the Co-SiO@sub 2@ and the Co-MgO systems whereas 500 ~ 1000 Oe of coercivities were observed in the Co-CoO films. AT 10 K the coercivity of the Co-SiO@sub 2@ film increased to 760 Oe while the coercivity of the Co-MgO and Co-CoO films increased to 6 kOe and 10 kOe, respectively. Unlike the Co-SiO@sub 2@ system, a small M-H loop shift was observed in the Co-MgO system at 10 K and disappeared above 50 K. This results indicated that there would be a small amounts of Co oxide phase existed in Co-MgO films and this may be the reason for the high coercivity at low temperature. In the Co-CoO system, the loop shifts were observed up to 250 K. In this presentation the magnetic properties of each film will be discussed based on the microstructural and magnetic effects from the different matrix.

Topical Conference on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics

Room 6C - Session NT+NS+EM+MS-ThM

Nanotubes: Nanoelectronics and Field Emission

Moderator: N.J. Halas, Rice University

8:20am **NT+NS+EM+MS-ThM1 Carbon Nanotube Molecular Electronics**, ***C. Dekker,*** Delft University of Technology, The Netherlands **INVITED**

I will present various recent results from electron transport measurements and scanning-probe microscopy on individual single-wall carbon nanotubes. Our early electrical transport work showed mesoscopic signatures at cryogenic temperatures. Additionally, a room-temperature transistor based on an individual semiconducting nanotube was established. Recent results in transport studies include first measurements on samples with low-ohmic contacts. The nanotubes are found to sustain very high current densities (~10^9 A/cm^2). I will show first measurements on kinked nanotubes, which act as an ontube intramolecular junctions. If time allows I may also present our results on AFM manipulation of nanotubes, and electrical measurements on manipulated nanotubes.

9:00am **NT+NS+EM+MS-ThM3 Electrical Transport in Single-Wall Nanotube Rings: Coherence and Localization**, *H.R. Shea, R. Martel,* ***Ph. Avouris,*** IBM T.J. Watson Research Center

Understanding electrical transport in carbon nanotubes is essential for their possible use in nanoelectronics. Furthermore single-walled carbon nanotubes (SWNTs) provide ideal model systems on which to test theories of transport phenomena in 1D-systems. Linear SWNTs, however, do not have self-folding electron trajectories which can enclose magnetic flux. Thus, the technique of magneto-resistance (MR) cannot be applied directly to obtain information on the mechanism of electrical transport. Recently, we have developed a procedure by which linear SWNTs can be induced to form ring structures. Despite the high flexural rigidity of these materials, coils stabilized only by van der Waals forces can be produced in yields of ~50 %. These rings provide an ideal geometry for MR measurements. The MR is negative over the range of 0-5 T and from it we are able to determine the coherence length of the electrons in the rings. We found that over the entire range of 3 K - 60 K the SWNT-rings are in a state of weak localization induced by the constructive interference of electron waves propagating in opposite directions around the ring. Electric transport is not ballistic, and the coherence length reaches 520 nm at 3 K. From the temperature dependence of the coherence length we determine that the dominant dephasing mechanism at low T involves electron-electron interactions (Nyquist mechanism). Below ~1 K we observe an electronic phase transition to a strongly localized state. This transition is accompanied by the opening of a small energy gap and very strong MR and universal conductance fluctuations. An interesting zero bias anomaly (ZBA) is also observed below ~0.7 K. This ZBA is sensitive to magnetic fields and is ascribed to Kondo-type scattering from localized magnetic moments.

9:20am **NT+NS+EM+MS-ThM4 Analysis of Carbon Nanotube Field-Effect-Transistors (FETs)**, ***T. Yamada,*** NASA Ames Research Center

Recent experiments on carbon nanotube FETs@footnote 1@ are analyzed theoretically. Comparing to the familiar Metal-oxide-semiconductor (MOS) FET characteristics, two qualitatively different behaviors can be pointed out:@footnote 1@ (1) the channel conductance g@sub d@ as a function of

gate voltage V@sub g@ is not linear but somehow saturates, and (2) the drain current I@sub d@ does not saturate with the drain voltage V@sub d@ but rather monotonically increases. As for g@sub d@(V@sub g@), a staircase-like curve is expected with possible rounding. Each time the Fermi energy crosses a degenerate new subband, the nanotube conductance increases by double the quantum conductance, and thus g@sub d@ forms steps. When moving up to a next step, one new additional degenerate subband needs to be filled in the inversion layer, where larger V@sub g@ has to be applied. This will be a mechanism for the g@sub d@ saturation. The absence of I@sub d@(V@sub d@) saturation is due to the infrequent inelastic scattering by phonons or other carriers in the channel, regardless of the frequent elastic scattering by defects or impurities determining the small g@sub d@ (1/g@sub d@ ~ 2.9 M@ohm@).@footnote 1@ Carriers are not thermalized in the channel without efficient inelastic scattering, resulting in no channel pinch-off formation and no I@sub d@ saturation. These reflect the nanotube electronic properties. We need to take them into account in the future device/circuit design, and develop a scheme best suitable for nanotube FETs. @FootnoteText@ @footnote 1@S.J. Tans, R.M. Verschueren & C. Dekker, Nature, 393, 49 (1998); R. Martel, T. Schmidt, H.R. Shea, T. Hertel, Ph. Avouris, Appl. Phys. Lett. 73, 2447 (1998).

9:40am **NT+NS+EM+MS-ThM5 Novel Length Scales in Nanotube Devices**, ***F. Léonard***, *J. Tersoff,* IBM T.J. Watson Research Center

We calculate the properties of p-n junctions, n-i junctions, and Schottky barriers made on a single-wall carbon nanotube. In contrast to planar bulk junctions, the depletion width for nanotubes varies exponentially with inverse doping. In addition, there is a very long-range (logarithmic) tail in the charge distribution, extending over the entire tube. These effects can render traditional devices unworkable, while opening new possibilities for device design. Our general conclusions should apply to a broad class of nanotube heterojunctions, and to other quasi-one-dimensional ``molecular wire" devices.

10:00am **NT+NS+EM+MS-ThM6 Field Emission from Carbon Nanotubes and Its Application to Electron Sources in Display Elements**, ***Y. Saito,*** Mie University, Japan*; S. Uemura,* Ise Electronics Corp., Japan **INVITED**

Carbon nanotubes posses the following properties favorable for field emitters: (1) high aspect ratio, (2) small radius of curvature at their tips , (3) high chemical stability and (4) high mechanical strength. Field emission microscopy was carried out for both multiwall nanotubes (MWNTs) and single-wall nanotubes (SWNTs) produced by arc discharge between carbon. Four kinds of nanotubes were investigated; viz., (1) as-grown MWNTs prepared in the helium arc (called "pristine MWNTs"), (2) as-grown MWNTs in hydrogen ("nanog rafibers"), (3) purified MWNTs with open ends ("purified MWNTs" or "open MWN Ts"), and (4) purified SWNTs. Field emission patterns as well as current versus voltage characteristics and Fowler-Nordheim plots for respective nanotubes will be discussed. As an application of nanotube field emitters, we manufactured cathode-ray tube (CRT) type lighting-elements and vacuum-fluorescence display (VFD) panels. In both display elements, conventional thermionic cathodes were replaced with MWNT field emitters which were fixed onto a stainless steel cathode by using conductive paste. In CRT-type lighting elements, the nanotube cold cathode was covered with a grid electrode, the gap between the cathode and the grid being in a range from 0.2 to 0.7 mm. Current density on the cathode surface was on the order of 10 - 100 mA/cm@super 2@ at an average field strength of 1.5 V/ µm. Luminance of the phosphor was intense enough for practical use; e.g., 6.3x10@super 4@ cd/m@super 2@ for green light at an anode current of 0.2 mA and an anode voltage of 10 kV. A direct-current driving test revealed a lifetime over 10,000 hours.

10:40am **NT+NS+EM+MS-ThM8 Emission Properties of Large-area, Fully-sealed Carbon Nanotube Field Emission Display**, ***W.B. Choi***, *H.Y. Kim, D.S. Chung, J.H. Kang, I.T. Han, J.M. Kim,* Samsung Advanced Institute of Technology, Korea

Fully sealed field emission display (FED) in size of 4.5 inch has been fabricated by using carbon nanotubes. Carbon nanotubes were fabricated by arc discharge technique. Carbon nanotube aligning techniques with the aid of slurry squeezing and electrophoresis were used for making large-area cathode. The Y@sub 2@O@sub 2@S:Eu, ZnS:Cu,Al, and ZnS:Ag,Cl, phosphors are deposited on the anode glass for red, green, and blue colors, respectively. The assembled structure was sealed in an atmosphere of highly purified Ar gas by means of a glass frit. The display plate was evacuated down to the pressure level of 1x10@super -7@ Torr. Three non-evaporable getters of Ti-Zr-V-Fe were activated during the final heat-exhausting procedure. Finally, the active area of 4.5-inch panel with fully sealed carbon nanotubes was produced. The turn-on field for lighting phosphor was 1.5 V/µm. Brightness of over 1000 cd/m@super 2@ at 4V/µm was achieved on the entire area of 4.5-inch panel from the green phosphor-ITO glass. The fluctuation of the current was satisfied for the field emission display. These reliable results enable us to produce carbon nanotube-based large area full-color FEDs in the near future. In this presentation, fabrication techniques and emission properties of large area carbon nanotube FED will be demonstrated.

11:00am **NT+NS+EM+MS-ThM9 The Structure of Nanotubes Observed with Thermal Field Emission**, ***K.A. Dean***, *B.R. Chalamala,* Motorola Flat Panel Display Division*; O. Groening, O.M. Kuettel,* University of Fribourg, Switzerland

We studied the structure of single-walled nanotubes (SWNTs) using field emission microscopy. The field emission images obtained after thermal cleaning depict the spatially-resolved electronic structure of the individual SWNT caps. Using high temperature field emission, we demonstrate how to distinguish between the patterns of individual SWNTs and those of clusters, how to alter the structure of the nanotube cap, and how to extract information about the SWNT structure and chirality from the field emission image. In addition, we demonstrate a technique for measuring the SWNT local density of states through thermal field emission energy distribution measurements. With this technique, we observe that nanotubes have discrete electronic states several eV above the Fermi level, and we suggest that these states are responsible for the large variation in emission current vs. temperature behavior observed among nanotubes.

11:20am **NT+NS+EM+MS-ThM10 Fabrication and Field Emission Properties of Adherent Carbon Nanotube Films**, ***C. Bower,*** University of North Carolina at Chapel Hill*; W. Zhu, G. Kochanski, S. Jin,* Bell Laboratories, Lucent Technologies*; O. Zhou,* University of North Carolina at Chapel Hill

We report on the fabrication and field emission properties of carbon nanotube films. Films of randomly oriented carbon nanotubes were deposited onto substrates using a variety of techniques. The nanotube films exhibited stable field emission current at low turn-on fields (electric field needed to generate 1 nA of current) and threshold fields (electric field needed to generate 10 mA/cm@super 2@). A single-walled carbon nanotube film with approximately 20% surface coverage showed a turn-on field of 1-1.2 V/µm and a threshold field of 1.3-1.7 V/µm. The emission characteristics deviated from typical Fowler-Nordheim behavior at high current densities. The nanotube films were capable of generating large current densities (> 4 A/cm@super 2@). The emission properties were found to be stable over several days of emitting at 10 mA/cm@super 2@. The emission site density of the films was measured to be 10@super 4@-10@super 5@ sites/cm@super 2@ and the emission patterns were studied.

11:40am **NT+NS+EM+MS-ThM11 Characterization of Oriented Carbon Nanotube Cathodes for Field Emission Flat Panel Display and Light Source Applications**, ***N.N. Chubun,*** SRPC Istok, Friazino, Russia*; A.G. Chakhovskoi, C.E. Hunt,* University of California, Davis*; A.N. Obraztsov,* Moscow State University, Russia

Oriented carbon nanotubes were recently reported as a viable material for fabrication of field emission cathodes applicable to flat panel displays and vacuum light sources.@footnote 1@ Field emission properties of diode and triode structures with oriented nanotube cathodes were studied in DC-mode in ultra-high vacuum chamber and in sealed glass prototype devices. Cathodes of 9x9mm grown using glow-activated direct current discharge CVD method on molybdenum and single crystal silicon substrates were studied at currents up to 2 milliamps using metal or phosphor coated anodes. The nanotubes exhibited various degrees of initial surface orientation depending on parameters of the deposition process. An additional orientation of the nanotubes in electric filed during first activation of the cathodes was observed. Monochrome low-voltage FPD phosphors were used for cathodoluminescent brightness/light efficiency characterization and for monitoring of distribution of the filed emission sites. Turn-on voltages varied from 1 to 5 V per micron depending on the extraction electrode configuration. Influence of vacuum conditions and initial training on stability and lifetime of the cathodes was studied. I/V characteristics of the nanotube cathodes were directly compared to those of carbon fiber and carbon foam emitters and to diamond-coated field emission arrays showing potentially greater reproducibility and uniformity of filed emission of the oriented nanotube cathodes. @FootnoteText@ @footnote 1@ A.N.Obraztsov, I.Yu.Pavlovsky, A.P.Volkov, V.L.Kuztetsov, A.L.Chuvilin. MRS 1999 Spring Meeting, San Francisco, CA, April 1999, p.B.4.9/C.2.9.

Surface Science Division
Room 607 - Session SS2+EM+NS-ThM

Nucleation and Growth

Moderator: G.M. Nathanson, University of Wisconsin, Madison

8:20am **SS2+EM+NS-ThM1 Evolving Surface Morphology: An In Situ STM Study of 2-20 nm SiGe Quantum Wells Grown on 75 mm Si (100) Wafers**, ***G.G. Jernigan,*** Naval Research Laboratory, US*; P.E. Thompson,* Naval Research Laboratory

Electrical device improvement will come from the understanding and control of interfaces at the atomic level. We have integrated an STM with a commercial Si MBE system for in situ examination of device structures grown on full 75 mm wafers. Our first system of study is the growth of SiGe quantum wells on Si (100). SiGe is being investigated for its use in optoelectronics and high speed circuits. We will present a description of the atomic surface morphology of the initial 100 nm epitaxial Si buffer layer, followed by a Si@sub 0.8@Ge@sub 0.2@ quantum well of thickness up to 20 nm, and a Si capping layer deposited after the quantum well. The Si buffer layer is grown using a 0.08 nm/s Si flux onto a 650 @super o@C substrate. Step-flow growth occurs, but the different adatom sticking probabilities at the S@sub A@ and S@sub B@ steps produces a "wavy" surface which is the result of alternating terraces growing rapidly in different directions rotated by 90@super o@. The deposition of Si@sub 0.8@Ge@sub 0.2@, by co-depositing Ge with a 0.02 nm/s flux and Si, disrupts the "wavy" growth morphology. Ge segregation during deposition produces a "2xn" surface reconstruction that consists of rows which run perpendicular (G@sub A@) and parallel (G@sub B@) to a step edge in a manner analogous to the S@sub A@ and S@sub B@ steps, respectively. The quantum well morphology consists of a mosaic of small terraces containing short rows of G@sub A@ steps and long rows of G@sub B@ steps. The Si capping layer grown on the quantum well reinstates the "wavy" morphology. However, in addition to the S@sub A@ and S@sub B@ step-flow growth, dimer vacancy lines are now observed within the S@sub A@ terraces and are due to Ge segregation from the quantum well. The effects of S@sub A@/S@sub B@ waves, Ge "2xn" terraces, and dimer vacancy lines as a function of growth rate and temperature will be discussed. This work was supported by the ONR.

8:40am **SS2+EM+NS-ThM2 Hydrogen-Mediated Surface Morphological Evolution in Si@sub 0.7@Ge@sub 0.3@/Si(001) Layers Grown by Hydride Gas-source Molecular Beam Epitaxy**, ***T. Spila,*** *P. Desjardins, H. Kim, N. Taylor, D.G. Cahill, J.E. Greene,* University of Illinois, Urbana*; S. Guillon, R.A. Masut,* Ecole Polytechnique de Montréal, Canada

The primary mechanisms for relieving misfit strain @epsilon@ during heteroepitaxy are the formation of misfit dislocations (MD) and strain-induced roughening. These mechanisms are initially competing (due to @epsilon@-dependent activation energies) and eventually interacting once relaxation is initiated. Si@sub 0.7@Ge@sub0.3@ layers were grown on Si(001) (miscuts @<=@ 0.1°) to quantitatively investigate the effects of Ge surface segregation and steady-state hydrogen coverage @theta@@sub H@ on mechanisms of surface morphological evolution during GS-MBE from Si@sub 2@H@sub 6@/Ge@sub 2@H@sub 6@. For growth temperatures T@sub s@ > 600 °C where @theta@@sub H@ = 0, layers exhibit (by AFM and XTEM) surface morphologies similar to that observed in solid-source MBE. The islanding process observed at T@sub s@ = 800 °C relieves 45% of the strain (determined from x-ray reciprocal lattice maps) without the introduction of MDs for thicknesses t up to 31 nm. The dominant facet planes evolve from {105}/{113} to {518}/{111}/{011} with increasing t until coalescence (t = 180 nm). Decreasing T@sub s@ < 600 °C to a regime where @theta@@sub H@ > 0 allows an opportunity to probe new hydrogen-mediated surface morphological pathways. The tendency toward strain-induced roughening and faceting decreases with decreasing T@sub s@ as the initial low-thickness strain-relaxation mechanism and corresponding in-plane feature size changes from strain-induced roughening to MD nucleation when T@sub s@ is decreased below 525 °C. We discuss the details of surface morphological evolution in each of the three temperature regimes (< 525, 525-600, and > 600 °C) in terms of local precursor adsorption and H-desorption kinetics.

9:00am **SS2+EM+NS-ThM3 Interdiffusion During Growth of Ge on Si(100)**, ***H. Jonsson,*** *B.P. Uberuaga, M. Leskovar, B.R. Schroeder, S. Meng, M.A. Olmstead,* University of Washington

We present both experimental evidence and a theoretical explanation of sub-monolayer Ge epitaxy on Si(100) interdiffusion to the 4th layer of the Si substrate. XPD measurements at both 500 C and 700 C show the presence of Ge atoms in the 4th layer. DFT/GGA calculations of the energetics of a Ge atom in the Si surface, together with a statistical model of Ge occupation of the lattice sites, predict occupation of sub-surface sites, with enhanced occupation in the sites under tensile strain. The calculations indicate that the formation energy of a Ge interstitial near the surface (about 1 eV higher energy than the adatom) is significantly reduced as compared with an interstitial in bulk Si, thus lowering the energy barrier for the interstitial diffusion mechanism near the surface. This work was supported by the National Science Foundation, the University of Washington Royalty Research Fund and the Japanese New Energy and Technology Development Organization.

9:20am **SS2+EM+NS-ThM4 Confined Intermixing of Ge and Si**, ***S.-J. Kahng,*** Seoul National University, Korea*; Y.H. Ha, D.W. Moon,* Korea Research Institute of Standards and Science, Korea*; Y. Kuk,* Seoul National University, Korea

In Ge-Si superlattice system, the efficiencies of a possible optoelectric and fast devices can be improved by optimizing the composition at each layer and the abruptness at the interface. It is well- known that intermixing between Ge and Si atoms mainly occurs during the growth process of Si layers on the previously grown Ge layers. Ge atoms tend to segregate toward the surface since the surface free energy of Ge is lower than that of Si. However, with hydrogen adsorbate, the surface free energy of Ge is lower than that of Si, possibly inducing segregation of Si in the Ge overlayer. In this study, Si surface segregation was studied quantitatively for the Ge overlayers grown on Si(100)-(2 x 1) with channeled medium energy ion scattering spectroscopy. The intermixing between Ge and Si presents only at the initial layer in the presence of hydrogen surfactant. Microscopic mechanism for the growth process will be discussed in the view point of kinetics as well as energetics.

9:40am **SS2+EM+NS-ThM5 Surface Segregation and Surface Reactivity in Heteroepitaxial Vapor Phase Thin Film Growth: Si@sub 1-x@Ge@sub x@ on Si(111)**, ***Y.-J. Zheng,*** *A.M. Lam, J.R. Engstrom,* Cornell University

Supersonic molecular beam scattering, x-ray photoelectron spectroscopy (XPS) and low-energy ion scattering spectrometry (LEISS) have been employed to examine the heteroepitaxial growth of Si@sub 1-x@Ge@sub x@ thin films on Si(111) surfaces. Molecular beam scattering has been employed to measure the reactivity of Si@sub 2@H@sub 6@ and GeH@sub 4@ on the Si@sub 1-x@Ge@sub x@ alloy surfaces for a variety of growth conditions (composition and substrate temperature), and these results are compared with results obtained on the clean Si(111) and Ge(111) surfaces. We find that the alloy surfaces are less reactive than both of the pure elemental Si and Ge surfaces. This is in stark contrast to our results for the (100) orientations, where alloy reactivity was always intermediate to that observed on clean Si and Ge. These results reflect the important role played by surface reconstructions on the (111) orientations. XPS and LEISS have been employed in situ to quantify the near-surface Ge concentration of the Si@sub 1-x@Ge@sub x@ epitaxial thin films. Ge segregation is significant, although somewhat less pronounced compared to what we have observed previously on the (100) orientations. Ge segregation, which occurs also in the subsurface layers, has been successfully modeled using both a statistical thermodynamic analytical model, and Monte Carlo simulations.

10:00am **SS2+EM+NS-ThM6 The Role of Arsenic Surfactant in the Growth of Germanium Thin Films on Si(100) Surfaces**, ***C.L. Berrie,*** *J. Bright, S.R. Leone,* University of Colorado, Boulder

The role of arsenic surfactant in the growth of germanium films on Si(100) substrates is investigated using laser single photon ionization time of flight mass spectrometry, reflection high energy electron diffraction, and atomic force microscopy. The energetics of arsenic interaction with Si(100) and Ge(100) are investigated by monitoring the temperature dependence of the desorbing fluxes of As@sub 4@, As@sub 2@ and As atoms from the substrate under a constant incident As@sub 4@ flux. These measurements indicate that the As@sub 2@ interactions with Si(100) and Ge(100) differ dramatically. In particular, the As@sub 2@ flux plateaus in the case of the Si(100) substrate from 800 K to 1000 K. In the case of the Ge(100) substrate, the As@sub 2@ flux monotonically increases over this temperature range and a similar plateau is not observed. Measurements of the desorbing As@sub n@ fluxes are also made during Ge growth on a Si(100) surface. The dramatic difference in the arsenic interaction on these two surfaces is evident in these measurements as well. The morphologies of the resulting films are monitored ex-situ using atomic force microscopy to determine the effect of arsenic coverage on the size and density distributions of islands formed. As the arsenic coverage is increases, the

observed island size decreases and the density of islands increases dramatically. The mechanisms for the Ge growth and the interaction in the presence of the arsenic surfactant will be considered.

10:20am **SS2+EM+NS-ThM7 The Dynamics of the Si(111) (7x7) to (1x1) Phase Transition Investigated by Low Energy Electron Microscopy**, ***J.B. Hannon,*** Carnegie Mellon University **INVITED**

We have used low-energy electron microscopy (LEEM) to investigate the dynamics of the (7x7) to (1x1) phase transition on the Si(111) surface. Because the density of the (1x1) surface is 6 percent larger than that of the (7x7) surface, the conversion from (7x7) to (1x1) requires transport of mass to the domain boundary. By measuring the time evolution of complicated configurations of triangular (7x7) domains, and comparing the results to detailed simulations, we are able to quantify the role of mass transport in the dynamics of this phase transition. We find that individual domains decay approximately linearly in time, with a decay rate determined, not by the domain size, but by the local arrangement of neighboring domains. This observation is counter to the simplest picture of phase boundary motion, in which domain walls move with a constant velocity (independent of environment) determined by the free energy difference between the two phases. We have modeled the effect of the mass transport requirement on the observed decay by solving the two-dimensional diffusion equation for the experimentally-observed configuration of 7x7 domains. We find that the (7x7) domain decay is indeed limited by the supply of the additional material to the boundary. Detailed comparison of the diffusion model with experiment suggests the surprising result that the terrace (rather than surface steps) acts as the primary source of the additional atoms required for the (7x7) to (1x1) conversion. This model reproduces the simultaneous decay of all islands in the field of view with only one adjustable parameter.

11:00am **SS2+EM+NS-ThM9 The Motion of Atomic Steps on Ultra-Flat Si(111)**, ***P. Finnie,*** *Y. Homma,* NTT Basic Research Laboratories, Japan

The flattest silicon surfaces are typically made up of terraces of a low index crystal plane connected by atomic steps. We have studied sublimation and growth on ultra-flat Si(111) substrates@footnote 1@ which have (111) terraces of up to 50 microns in width separated by monoatomic steps. The motion of atomic steps is revealed in time lapse movies made by in situ scanning electron microscopy. When samples are heated to high temperatures (about 1000°C) the surface erodes in a step-flow mode: steps retreat in an orderly fashion, one after the other. Since new terraces are nucleated when step spacings exceed a temperature dependent critical length, the spacing between steps is tunable. Measurements of step velocities as a function of terrace width compare well with theory. The interactions between steps are observed directly by forcing steps to collide@footnote 2@ either destructively, in which opposing steps annihilate, or constructively, in which steps moving in tandem coalesce into double (or triple, or larger) steps. We also studied molecular beam epitaxy in this high temperature regime. Using an electron beam to supply a flux of elemental silicon, desorption is countered and growth occurs in the step-flow mode. Remarkably flat grown surfaces can be obtained in this way since step-flow growth maintains an ultra-flat profile. Monoatomic height island nucleation can also be observed, with circular islands growing to diameters of tens of microns, seamlessly merging with neighboring terraces as the steps collide destructively. @FootnoteText@ @footnote 1@ Y. Homma, H. Hibino, T. Ogino, and N. Aizawa, Phys. Rev. B 55 (1997) R10237 @footnote 2@ P. Finnie and Y. Homma, Phys. Rev. Lett. 82 (1999) 2737.

11:20am **SS2+EM+NS-ThM10 Novel Growth Behavior of Ge on Pb Covered Si(111) Surface**, *I.S. Huang,* Academia Sinica, ROC; *T.C. Chang,* Academia Sinica, ROC, Republic of China; ***T. Tsong,*** Academia Sinica, ROC

A surfactant can modify the growth behavior of a system to our advantages. We report discovery of a novel growth behavior in a Pb-layer promoted growth of Ge on Si(111). For this system, not only can Ge atoms grow on Si(111) surface layer by layer for many layers, but the growth behavior is contrary to traditional nucleation and growth theory and most experimental results in epitaxy. This growth is not governed by the reaction-limited-aggregation (RLA) process at low temperature as has been found in traditional epitaxy. The most interesting feature we find is that a compact-to-fractal island shape transition occurs when the sample temperature is increased, or the deposition flux is decreased. In traditional epitaxy, fractal growth occurs by diffusion-limited-aggregation (DLA) at low temperatures, thus fractal growth will disappear as the sample temperature is raised to the extent that step edge diffusion can occur. Our observation demonstrates that fractal islands can also be grown by RLA, and the importance of reactions in aggregation of Ge atoms in this system. Earlier theories neglect the reaction processes which may be acceptable for metal-on-metal systems, but are not good enough for other systems. Our result points to a need to develop a more complete nucleation theory where both diffusion and reaction are properly taken into account.

11:40am **SS2+EM+NS-ThM11 The Growth of High Density, Small Ag Islands at the Si(111)7x7 Surfaces with Adatom Defects**, ***H. Hirayama,*** *H. Okamoto, K. Takayanagi,* Tokyo Institute of Technology, Japan

We studied the growth of Ag islands on the Si(111)7x7 surfaces with missing adatoms. The missing adatoms were created by 0.5keV Ar ion bombardment. Ag atoms were deposited on the surfaces at room temperature. The growths were observed by using scanning tunneling microscope (STM). At the Si(111)7x7 surface of no missing adatoms, several half unit triangular cells of the 7x7 reconstruction changed their contrast to be bright in the initial stage of the Ag deposition . Then, at the coverage above 0.03 monolayer (ML), each bright triangular cell changed to a bright spot. With the coverage, the number of bright spots increased, and occasionally two spots in neighboring cells kissed. At 0.8ML, the surface was covered by the two-dimensional (2D) percolating network of kissing spots. On the network, three-dimensional (3D) Ag islands grew. Meanwhile, at the Si(111)7x7 surfaces with missing adatoms, the bight spots appeared at the very early stage of the Ag deposition. The spots appeared as to avoid missing adatom sites. This resulted in an imperfect 2D network; the connection of kissing spots were cut into pieces here and there. On the imperfect 2D network, 3D islands grew above 0.7ML. At the stage of the 3D island growth, the missing adatom sites of the underlying 2D network was never filled up. However, we found strong dependence of the size and density of the 3D islands on the number of missing adatoms at the starting surfaces. With an increase of missing adatoms, the size of the islands decreased, while the density increased dramatically. The effects of the missing adatoms on the 3D Ag islands growth were attributed to the substantial increase of the super saturation and the decrease of the diffusion constant of Ag atoms on the imperfect 2D network.

Surface Science Division
Room 604 - Session SS3+AS+NS-ThM

Novel Surface Probes & Technique Enhancement

Moderator: B.E. Koel, University of Southern California

8:20am **SS3+AS+NS-ThM1 Determination of Sticking Probability and Transition State Energy by Line-of-Sight Detection: Halocarbons on Cu(111)**, ***A.S.Y. Chan,*** *C.A. Clifford, R.G. Jones,* University of Nottingham, UK

We have used a new technique, Line-of-Sight Sticking Probability (LOSSP) to study the reactions of chloroform and 1-bromo-2-chloroethane (BCE) on Cu(111). The sticking probability measurements were made by applying a thermally randomised pressure of the halocarbon above the surface and detecting the reflected flux as a narrow beam of molecules flying in line-of-sight from the centre of the sample surface to the mass spectrometer.@footnote 1@ The general reaction undergone by both halocarbons on the copper surface is: M(gas) -> M(phys) [1] M(phys) -> M(gas) [2] M(phys) -> chemisorbed halogens + gas phase product [3]. By measuring the sticking probability as a function of temperature, we are able to obtain the energies of the transition state M(phys) towards decomposition, which for the non-activated adsorption system of BCE on Cu(111) is ~13 kJ/mol below zero, and for the activated adsorption of chloroform on Cu(111) is ~4 kJ/mol above zero. (Zero energy is defined as the energy of the molecule at an infinite distance from the surface. @FootnoteText@ @footnote 1@ R G Jones and C J Fisher; Surface Science 424 (1999)127.

8:40am **SS3+AS+NS-ThM2 Demonstration of Angle Resolved Auger-photoelectron Coincidence Spectroscopy from a Solid: First Results from the Cu(111) Surface**, ***D.A. Arena,*** *R.A. Bartynski,* Rutgers University; *D. Cvetko, L. Floreano, A. Morgante, F. Tommasini,* Laboratorio Nazionale TASC-INFM, Italy; *A. Attili, A. Ruocco, G. Stefani,* Universita' di Roma, Italy; *L. Marassi, P. Luches,* Universita' di Modena, Italy; *S. Iacobucci,* CNR-IMAI, Montelibretti, Italy

We report the first successful angle-resolved Auger-photoelectron coincidence spectroscopy (AR-APECS) measurements from a solid. These measurements were made at the ALOISA beamline at the ELETTRA synchrotron radiation center in Trieste, Italy. This novel analysis chamber is equipped with seven hemispherical electron energy analyzers mounted on two independent rotatable frames; the arrangement allows for the efficient exploration of different kinematical conditions for the emitted pair of electrons. We measured the angular distribution of Cu L@sub3@VV

Auger electrons from the Cu(111) surface in coincidence with Cu 2p@sub 3/2@ photoelectrons emitted at selected angles; these angles correspond to maxima and minima in the photoelectron diffraction (PED) pattern. When the 2p@sub 3/2@ core level is at a PED maximum, the Auger pattern is indistinguishable (within statistics) from the noncoincidence distribution. In contrast, if the 2p@sub 3/2@ photoelectrons are at a PED minimum, the coincidence Auger angular distribution shows additional structure as compared to the noncoincidence pattern. This observation may arise because the two coincidence conditions access different intermediate states. The effects of the lattice may be more pronounced in the Auger angular pattern collected in coincidence with photoelectrons on the PED maximum while the Auger angular distribution acquired in coincidence with the photoelectrons on the PED minimum may exhibit more "atomic-like" behavior. Alternatively, the difference may be a consequence of different probing depths on and off the PED maximum, and hence the sampling of different scattering sites. Experiments to discriminate between these possibilities are currently underway. This work is supported by NSF-DMR 98-01681 and NATO-CRG 97-0175.

9:00am **SS3+AS+NS-ThM3 Multiple Atom Resonant Photoemission: A New Tool for Determining Near-Neighbor Atomic Identities and Bonding**, ***A.W. Kay***, UC Davis and LBNL; *E. Arenholz,* LBNL and UC Berkeley; *B.S. Mun,* UC Davis and LBNL; *J. Garcia de Abajo,* LBNL; *C.S. Fadley,* UC Davis and LBNL; *R. Denecke, Z. Hussain, M.A. Van Hove,* LBNL

A newly discovered resonance photoemission process between neighboring atoms in multielement samples will be presented. Experimental evidence for the effect and possible applications will be considered. In several metal oxides, including MnO, Fe2O3, and La0.7Sr0.3MnO3, we have observed an enhancement in the core-level photoelectron peak intensity associated with one element in the sample (e.g. O 1s) while the excitation energy is tuned through an energetically deeper absorption edge of a second element (e.g. Mn 2p or Fe 2p or La 3d). At the edges of this second element, a 40-100% enhancement in the peak intensity (as an area above inelastic background) of the first element is observed. Furthermore, this peak intensity enhancement exhibits a dependence upon photon energy that closely, but not identically, follows the x-ray absorption coefficient of the second atom. This is evidence of an interatomic or multi-atom resonance photoemission (MARPE) process, that is related to but distinctly different from the much-studied intraatomic or single-atom resonance photoemission (SARPE). Theoretical calculations based on extensions of previous intratomic resonance models have yielded encouraging agreement with our experimental results. The MARPE effect is expected to provide a direct method for determining the atomic identities (atomic numbers) of near-neighbor atoms to the excited atom, as well as providing a new technique for studying bonding and magnetism in molecules, at surfaces,buried interfaces, and perhaps bulk materials provided that secondary fluorescence detection of the resonance can be utilized.@footnote 1@ @FootnoteText@ @footnote 1@ This work was supported by the U.S. Department of Energy, Office of Energy Research, Basic Energy Sciences Division, Materials Science Division, and the Miller Institute (Berkeley).

9:20am **SS3+AS+NS-ThM4 Incident Beam Diffraction in Electron Stimulated Desorption**, ***M.T. Sieger***, *G.K. Schenter, T.M. Orlando,* Pacific Northwest National Laboratory

The use of electron beams to remove surface-bound atoms and molecules (electron-stimulated desorption, or ESD) is a topic of interest for many disciplines, from semiconductor device processing to astrophysics. We have been studying the role of scattering and diffraction of the incident electron in the initial state of the desorption process. We report calculations and experiments demonstrating that total ESD yields show fine-structure with incident electron direction, consistent with quantum-mechanical scattering and interference of the electron in the initial state of the desorption process. In a time-independent picture interference of the incident plane wave with waves scattered from the crystalline lattice forms an electron standing wave (ESW), having spatially localized maxima and minima in the incident electron density. Whether a particular point on a surface experiences a maximum or minimum depends on the wavelength of the electron, the direction of incidence relative to the crystal axes, and the locations of nearest neighbor atoms. Since the probability of excitation is proportional to the incident electron density at or near the site of the "absorber" atom (the site of the inelastic scattering event), the total ESD rate should depend upon the local atomic structure and the k-vector of the incident wave. The total desorption yield, when measured as a function of incident direction at constant energy, shows oscillations with the symmetry of the absorber bonding site. Since every inequivalent atomic bonding site has a unique pattern of oscillation electron standing wave stimulated desorption (ESWSD) measurements can in principle uniquely determine the bonding geometry of the absorber. We present experimental measurements for chlorinated Si surfaces.

9:40am **SS3+AS+NS-ThM5 Direct Atomistic Observation of Structural Dynamics in Surfaces and Interfaces by Time-Resolved High-Resolution Transmission Electron Microscopy**, ***T. Kizuka***, Nagoya University and Japan Science and Technology Corporation, Japan **INVITED**

Atomic processes of mechanical interaction and gas-phase epitaxial growth were directly observed in situ by time-resolved high-resolution transmission electron microscopy at spatial resolution of 0.1 nm and time resolution of 1/60 s. Nanometer-sized tips of gold and silicon approached, and were contacted, bonded, deformed and fractured inside a 200 kV electron microscope using a piezo-driving. Contact boundaries of a few atomic columns width in gold, silicon/silicon-oxide/silicon tunnel junctions, and quantum dots of silicon/gold-cluster/silicon were produced.@footnote 1@ A few layers near the surfaces and contact-boundaries were responsible for the bonding and separation processes. Atomic scale contact or non-contact type surface-scanning similar to that in scanning probe microscopy was performed by the same method.@footnote 2@ The mechanical removal of one atomic layer was also demonstrated.@footnote 3@ New kinds of atomic scale mechanical tests, such as friction test, compressing, tensile and shear deformation tests were proposed. Gold was vacuum-deposited on (001) surfaces of magnesium oxide inside the electron microscope. Atomic process of epitaxial growth was in-situ observed cross-sectionally. Various types of growth phenomena, such as 'embryo' formation, structural fluctuation, repeated process of truncation and construction of a corner in one gold cluster, secondary nucleation and coalescence, were analyzed in real-space.@footnote 4@ @FootnoteText@ @footnote 1@T. Kizuka, Phys. Rev. Lett., 81 (1998) 4448. @footnote 2@T. Kizuka et al., Phys. Rev., B55 (1997) R7398. @footnote 3@T. Kizuka, Phys. Rev. B57 (1998) 11158. @footnote 4@T. Kizuka et al., Phys. Rev. B56 (1997) R10079.

10:20am **SS3+AS+NS-ThM7 Ionization Mechanisms of Water in High Interfacial Electric Fields**, ***D.L. Scovell***[1], University of Washington, U.S.A; *V.K. Medvedev, C.J. Rothfuss, E.M. Stuve,* University of Washington

High surface fields (Ã1 V/Å) drive many important processes, such as electrochemistry and field emission. The behavior of water in these fields is important because water is the primary component in electrochemical processes and a major contaminant in the vacuum surrounding field emitter arrays in flat panel displays. It is usually assumed that water amplifies the field at the electrode surfaces, but little is known about how water affects the electric field distribution. Field emitter tips lend themselves to the study of the dielectric properties of water because they produce fields as high as 5 V/Å. To better understand the effect of high electric fields on water, numerical analyses have been conducted to model the electric field distribution around a water-covered emitter tip. The calculations include the field-dependence of the relative permittivity of the water adlayer. The model predicts that the dominant field occurs at the vacuum interface in thin water layers and at the metal surface in thick layers. In very thick layers the field at the tip surface is predicted to be greater than the applied electric field. This response is analogous to that assumed for a traditional electrode/electrolyte interface. Experiments have been conducted to verify the predicted trends for thin water layers. In these experiments water was adsorbed onto a platinum field emitter tip under field-free conditions in ultrahigh vacuum. Ionization was examined by isothermal ramped field desorption (RFD) performed as a function of temperature and water layer thickness. The experimental results are consistent with the predicted trends. This work was supported by the Office of Naval Research.

10:40am **SS3+AS+NS-ThM8 Free Electron Laser Nanospectroscopy Interface Applications**, ***G. Margaritondo***, Ecole Polytecnique Fédérale, Switzerland; *A. Cricenti,* Consiglio Nazionale delle Ricerche, Italy; *N.H. Tolk,* Vanderbilt University; *R. Generosi, P. Perfetti,* Consiglio Nazionale delle Ricerche, Italy; *I.D. Aggarwal,* U.S. Naval Research Laboratory

We present the first result of a major effort to investigate the lateral fluctuations of properties of solid interfaces on a microscopic scale. The key elements were the use of a small-tip optics fiber and its coupling with a scanning module; in this way, we achieved and verified the condition of near-field microscopy -- including a lateral resolution much below the wavelength value. Our discussion includes a presentation of the first

[1] **Morton S. Traum Award Finalist**

scanning near-field optical microscopy images obtained with a free electron laser infrared sources and data on small and microscopic-scale fluctuations of semiconductor interface barriers.

11:00am **SS3+AS+NS-ThM9 Imaging and Charge Transport Measurements using Dual-Probe Scanning Tunneling Microscopy**, ***H. Grube***, *J.J. Boland,* University of North Carolina

Scanning tunneling microscopy has evolved into a valuable tool for the study of semiconductor and metal surfaces. However, the single probe geometry of STM limits its application to local and static measurements of the local density of states.@footnote 1@ Incorporation of a second electrically and mechanically independent STM tip within nanometers of the first enables measurements of surface properties that conventional STM cannot perform.@footnote 2,3,4@ Our DP-STM has been characterized by placing both tips in close proximity on a sample surface and obtaining images from each tip showing its local surface environment and the other probe. We discuss the challenges encountered of DPSTM and the feasibility of charge transport measurements on a variety of systems including carbon nanotubes. @FootnoteText@ @footnote 1@ G. Binnig et al., Phys. Rev. Lett., 49 (1), 57 (1982)@footnote 2@ Q. Niu, M. C. Chang and C. K. Shih, Phys. Rev., B 51 (8), 5502 (1995)@footnote 3@ J. M. Beyers and M. E. Flatte, Phys. Rev. Lett., 74 (2), 306 (1995)@footnote 4@ J. M. Beyers and M. E. Flatte, J. Phys. Chem. Solids., 56 (12), 1701 (1995)

11:20am **SS3+AS+NS-ThM10 The Miniature Cylindrical Mirror Analyzer: A New Tool For Surface Analysis**, ***K. Grzelakowski***, Focus Polska Sp. Z o.o., Poland; *M.S. Altman,* Hong Kong University of Science and Technology, P.R. China

The design and performance of a new miniature cylindrical mirror analyzer (CMA) are presented. The CMA comprises outer and inner cylinders, integral on-axis electron gun, and detector system consisting of ring aperture and channeltron, all mounted on a 2.75" flange. Entrance angle, sample-to-detector distance, and polar cone angle were chosen, in consideration of second order focussing effects, that optimized analyzer transparency and resolution. Fringe field correction at the ends of the CMA is made by means of six rings precisely separated by sapphire insulators. The electron gun is a one-lens electrostatic system equipped with XY-deflector for beam adjustment and scanning. A CeB6 low temperature cathode operating at up to -2.0keV delivers emission current up to 100 mA. The energy range of analyzed electrons can be varied between 0 eV to 2.0 keV. The flange mounting also incorporates a high precision Z-motion for optimization of the working distance. The control electronics and software permit operation of the instrument in pulse and phase sensitive detection modes. Results obtained for a W(001) surface with this new miniature CMA demonstrate an energy resolution of 0.08%, which is comparable to larger 6" and 8" flange mounted instruments. The very small size of the mini-CMA permits its use in small or crowded ultra high vacuum chambers or where only 2.75" ports are available, thereby increasing flexibility in surface analysis.

11:40am **SS3+AS+NS-ThM11 Investigations of Surface Reactions on Thin Film-Supported Catalysts Using Microhotplate Arrays**, *R. Walton, R. Cavicchi,* ***S. Semancik***, *M. Class, J. Allen, J. Suehle,* National Institute of Standards and Technology

This presentation describes the use of microhotplate arrays and electrical measurements for efficiently investigating surface reactions on supported metal catalysts under varied temperature and gas exposure conditions. Each ~100 µm x 100 µm microhotplate platform used in our work includes functionality for rapid control and measurement of film temperature (thermal time constant ~ 1 ms) and for probing of gas-induced changes in a film's electrical properties. Arrays of individually addressable microhotplates are well suited for directly comparing catalytic layers of different composition, loading, and degree of dispersion. The results we present are relevant to both gas sensing and catalysis. Specifically, four-element arrays were used to evaluate reactions on Pt, Pd, and Cu catalyst particles (formed by annealing 25-100 Å layers) supported on tin oxide. Electrical conductivity was used to monitor changes in the electron density of the thin film catalysts caused by surface reactions in air of H@sub 2@, CO and CH@sub 3@OH, respectively, at film temperatures ranging from 20 to 500 °C. Each of the catalysts interacts with these reactants in air to produce changes in film conductivity that we relate to factors including surface oxygen concentration, reaction rates, catalyst loading, and catalyst fouling. As a further example of this approach, we also illustrate the use of microhotplates to explore the conditions of thermal cycling and partial pressures under which CO oxidation oscillations occur on Pt particles supported on SnO@sub 2@.

Magnetic Interfaces and Nanostructures Technical Group
Room 618/619 - Session MI+NS-ThA

Magnetic Imaging

Moderator: P.N. First, Georgia Institute of Technology

2:00pm **MI+NS-ThA1 Cryogenic Magnetic Force Microscopy Instrumentation**, ***M. Roseman***, *P. Grutter,* McGill University, Canada

We describe our cryogenic magnetic force microscope, operating between 4 and 300 Kelvin. The instrument is designed to fit within a 3" diameter bore of an 8 Tesla magnet. Cooling is achieved through the use of He exchange gas, which is pumped out prior to imaging in order to provide a vacuum of better than 10@super -5@ mbar during operation. The instrument uses a fibre optic interferometer to measure cantilever deflections. Through the use of a phase lock loop, this interferometric signal allows for the tracking of the cantilever resonant frequency with a resolution of 0.25 Hz in a 100 Hz measurement bandwidth. Our cantilevers are commercially available, made of single crystal silicon coated with a magnetic film, and routinely exhibit Q-factors of greater than 100,000 at 4 Kelvin. Piezoelectric-based clamping linear positioners, with step sizes of 50 nm (at 77 Kelvin) and capable of operation in high magnetic fields, perform in-situ tip and fibre approaches. As an effective means of vibration isolation, we suspend the microscope from a soft bellows. Comprised of 70 convolutions, the bellows damps out vibrations by more than an order of magnitude, effectively isolating the microscope from the surrounding environment, including pump vibrations and liquid helium boil-off. Particular attention has been paid to optimizing the signal to noise ratio through a systematic study of various noise sources, with the intent of achieving a thermally limited sensitivity.

2:20pm **MI+NS-ThA2 Modified Tips for High Resolution In-plane Magnetic Force Microscopy**, ***L. Folks***, IBM Almaden Research Center*; J.N. Chapman,* University of Glasgow, UK*; M.E. Best, P.M. Rice,* IBM Almaden Research Center*; B.D. Terris,* IBM Almaden Research center*; D. Weller,* IBM Almaden Research Center

Commercial batch-fabricated coated MFM tips have been modified to allow high resolution imaging of the in-plane components of stray field above a sample. A hole of diameter ~ 20nm was milled through the magnetic coating layer to the underlying silicon at the apex of each tip with a focussed gallium ion beam. The tips were then magnetized in the direction parallel to the sample plane. The hole at the apex forms a small pole gap and it is the interaction of the stray field from this gap with the sample stray field which produces the MFM signal. Accordingly, the resolution achievable is determined by the diameter of the hole milled at the apex. Note that such a controlled modification of the magnetic tip coating was suggested by Hill.@footnote 1@ High and low density data tracks, with transition spacings ranging from 1 micrometer to 50 nanometers, written in longitudinal granular recording media have been used to demonstrate the utility of the tips. By comparison of experimental results with simple theoretical models it is shown that the tips are strongly sensitive to the in-plane components of stray field. Furthermore, the modified tips exhibit better resolution than the unmodified tips, as may be seen from a side-by-side comparison of data collected from high density written transitions. The modified tips offer an inexpensive route to high resolution imaging of stray fields associated with in-plane domain structures. Hence they are of particular value for high density magnetic recording media investigations since the in-plane component of stray field is closely related to the signal detected by the recording head. @FootnoteText@ @footnote 1@ E. W. Hill, IEEE Trans. Magn. 31, 3355 (1995).

2:40pm **MI+NS-ThA3 Progress Toward Achieving Single-Spin Force Detection**, ***B.C. Stipe***, *D. Rugar, H.J. Mamin, C.S. Yannoni,* IBM Almaden Research Center*; T.D. Stowe, T.W. Kenny,* Stanford University

Magnetic resonance force microscopy was originally proposed@footnote 1@ as a method for imaging individual electron or nuclear spins. This talk will focus on recent progress toward achieving the necessary force sensitivity, tip field gradient, and spin lifetime to detect a single electron spin under real experimental conditions (i.e., with a sharp, submicron-size magnet mounted on an ultrasensitive cantilever within 100 Å of a sample surface). Characterization of the magnetic tip is especially important since the field gradient from the tip determines of the force from the spin. In addition, the spin relaxation rate can increase in the presence of magnetic field fluctuations from the tip. We have characterized the magnetic fluctuations of the tip at the cantilever frequency based on field dependent dissipation measurements on both Co thin film and NdFeB particle tips. NdFeB tips showed greatly reduced dissipation/fluctuations due, in part, to their high crystalline anisotropy. These tips should generate field gradients greater than 3 G/Å at the target spin, resulting in a force of more than 30 aN. Using custom fabricated single crystal silicon cantilevers at 2.5 K, we have achieved a force resolution of 2.8 aNHz@super -1/2@ far from the sample surface. However, within 500 Å of the sample, tip-surface interactions can significantly increase the force noise and cantilever frequency jitter. The origin of these effects and methods for reducing them will be discussed. This work is supported, in part, by the Office of Naval Research. @FootnoteText@ @footnote 1@ J.A. Sidles, Phys. Rev. Lett. 68, 1124 (1992).

3:00pm **MI+NS-ThA4 Magnetic Imaging by Spin-polarized Scanning Tunneling Microscopy**, ***W. Wulfhekel***, *J. Kirschner,* MPI fur Mikrostrukturphysik Halle, Germany

A new approach to spin-polarized scanning tunneling microscopy based on the magneto tunnel effect between a ferromagnetic tip and a ferromagnetic sample is demonstrated. By periodically changing the magnetization of the tip in combination with a lock-in technique, topographic and spin-dependent parts of the tunnel current are separated. This allows to simultaneously record the topography and the magnetic structure of the sample. First results are given for polycrystalline Ni and single crystalline Co(0001) surfaces, revealing a high spin contrast of up to 20% of the tunneling current, low data acquisition times of few ms/pixel and a resolution down to 10nm. The magnetic origin of the observed signal is proven rigorously by recording the domain wall motion due to an applied magnetic field during scanning. Potentials and limitations of this new technique are discussed.

3:20pm **MI+NS-ThA5 Spin-Polarized Scanning Tunneling Spectroscopy: Magnetic Domain Imaging and Beyond**, ***R. Wiesendanger***, *M. Bode, M. Getzlaff,* University of Hamburg, Germany **INVITED**

Spin-polarized vacuum tunneling from ferromagnetic thin film probe tips into exchange-split surface states of rare-earth thin films is demonstrated and applied to magnetic domain imaging with a spatial resolution below 20 nm. The bias dependence of the spin polarization extracted from tunneling spectroscopy data is found to be in surprisingly good agreement with results from spin-resolved (inverse) photoemission indicating that spin-dependent density-of-states effects dominate over matrix element effects. It is also shown that spin-polarized electronic states can yield high tunneling magnetoresistance. On the other hand, surface contamination leads to a strong decrease of the measured spin-polarisation by impurity-assisted scattering which influences strongly the vacuum-TMR effect as well as the contrast in spatially resolved magnetic imaging applications.

4:00pm **MI+NS-ThA7 Scanning-aperture Photo-emission Microscope for Magnetic Imaging**, ***G.M. McClelland***, *C.T. Rettner,* IBM Almaden Research Center

We have demonstrated a new technique for magnetic imaging that is ultimately capable of spatial resolution better than 5 nm. In our instrument, photoemission is excited by a laser focused to a 10-micron spot. A scanning aperture above the magnetic surface allows only electrons from a small selected region to reach the electron detector. The magnetization in this region is determined from the dependence of photoemission on the circular polarization of the laser. Images of 10-nm-thick Co-Pt multilayer thin films on sapphire have been obtained. From a cesiated film, a high quantum efficiency of 0.002 was observed from 458 nm laser light. Circular dichroism of +/- 2 % is recorded by alternating the circular polarization of the light while scanning. The tip distance above the surface is maintained by advancing the tip until 1-nA tunneling to a positive sample is observed, then withdrawing 15 nm and switching polarity to detect photoemission through the tip. The resolution we observe agrees well with the 35-nm-sized aperture in the gold tip. From the observed noise, we project that there is enough signal to image at 5 nm resolution if a small enough aperture can be fabricated. Recent calculations show that image forces on the electron from the aperture walls act to make the effective aperture even smaller than the physical diameter. The insensitivity of the instrument to varying magnetic fields should make it ideal for time dependent magnetization measurements in an applied field.

4:20pm **MI+NS-ThA8 Magnetic and Chemical Microanalysis Using SEMPA and SAM**, ***G. Steierl,*** *W. Lutzke, H.P. Oepen, J. Kirschner,* Max-Planck-Institut für Mikrostrukturphysik, Germany

Industrial demands led to an enormous interest in micromagnetic analysis tools that can be applied to a wide range of samples including lithographically produced samples with complex chemical compositions. To meet these requirements a new instrument was designed that combines Scanning Auger Microscopy (SAM) and Scanning Electron Microscopy with Polarization Analysis (SEMPA). The core elements are a Schottky thermal field emitter electron gun with coaxial cylindrical mirror analyzer (PHI-SAN 670), a retractable electron-lens system and a spin detector based on Spin Polarized Low Energy Electron Diffraction (SPLEED). The characteristics of these core elements are described and the performance of the entire system is demonstrated by high-resolution chemical and magnetic analysis of Ni@sub 80@Fe@sub 20@- and Co elements. The microstructures of 50nm thickness were produced by using electron beam lithography and lift-off. Oxidized Si(111)-wafers were used as substrate material with an oxide layer thickness ranging from about 10nm (natural oxide layer) to 1200nm (thermally oxidized). It is demonstrated that the electrical insulation of the microstructures due to the oxide-layer does not impede high resolution domain microscopy, if suitable surface preparation techniques are used. Several details of the domain patterns encountered in microstructures of different geometry (squares, rectangles, disks) and of lateral length ranging from 500nm to 10 µm are reported.

4:40pm **MI+NS-ThA9 Low Temperature Magnetic Domain Imaging with Spin Polarized Low Energy Electron Microscopy**, ***E.D. Tober,*** NCEM, Lawrence Berkeley National Laboratory*; G. Witte,* Ruhr-Universität Bochum, Germany*; H. Poppa,* NCEM, Lawrence Berkeley National Laboratory

Spin Polarized Low Energy Microscopy (SPLEEM) has for the first time been employed to examine magnetic surfaces below room temperature. With the recent addition of a liquid nitrogen based cooling stage for our instrument, we have the ability to achieve sample temperatures in the range of 110 - 2200 K. SPLEEM has the advantages of high spatial resolution (~10.0 nm) and atomic height resolution combined with image acquisition at near video rates. A full description of the system design as well as its application in exploring the magnetic domain formation in thin films of Co grown in situ on Pt(111) and Au(111) surfaces will be presented.

5:00pm **MI+NS-ThA10 Ballistic Electron Magnetic Microscopy: Imaging Magnetic Domains with Nanometer Resolution**, ***W.H. Rippard***[1], *R.A. Buhrman,* Cornell University

A new magnetic imaging technique with nanometer resolution, ballistic electron magnetic microscopy (BEMM), is introduced and used to image magnetic structure in copper-cobalt multilayer films. Magnetic domains are clearly observed and are found to give more than 300% contrast in the resulting BEMM images. Domain wall motion is also studied as a function of applied magnetic field. Magnetic contrast is observed on length scales of less than 100 nm and fluctuations of the ballistic transport in the system are observed on scales of less than 10 nm. The magnetic contrast is found to be strongly dependent on magnetic layer thickness while only weakly dependent on the number of layers in the multilayer stack. An energy dependent difference in the electron transport as a function of the relative alignment between the magnetic layers is also reported, revealing the effects of the Co band structure on the ballistic current transport. Strong magnetic contrast is observed at energies as high as 4 eV, demonstrating a large asymmetry in the effective spin-dependent mean free paths in this system. The local nature of the technique also allows the direct imaging of the effects of interfacial dopants on the ballistic transport in the multilayer films. Results from such dusting studies are also presented.

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

Nanotubes: Functionalization and Metrology

Moderator: D. Herr, Semiconductor Research Corporation

2:00pm **NT+NS+EM+MS-ThA1 Opportunities and Challenges for Nanotubes in Future Integrated Circuits**, ***R.R. Doering,*** Texas Instruments **INVITED**

We speculate about a few potential research opportunities that may be of mutual interest to both the microelectronics and nanotube communities. Perhaps the most evolutionary use of nanotubes in integrated circuits would be in the form of "thin films." Such use would capitalize on "bulk" material properties. For example, a layer of nanotubes (with "best metallic" conductivity) might serve as an interconnect film. Alternatively, an insulating nanotube layer (e.g, "modified" CNTs or other tube chemistries) might be used as a low-K dielectric. Even lower K might be achieved by using high-conductivity CNTs as "self-supporting wires," taking advantage of their inherent mechanical strength to eliminate the need for solid insulating layers. Another type of evolutionary use might involve nanotube structures for passive IC components. For example, the huge volume density of surface area looks appealing for DRAM capacitors. A significant amount of current nanotube research is aimed at active devices, which might ultimately replace today's silicon semiconductor switches. One of the most exciting prospects is the potential for more extensive and effective use of the "third-dimension" in integrated circuits. However, as with today's "planar" IC technology, the benefit/cost of "going 3D" will depend on details of the practical fabrication techniques. For nanotubes, this brings up "formation/place/route" issues. Nanotubes may also play a role in future "atomically perfect manufacturing," which may be needed to scale much below about 50-nm features regardless of the type of device technology employed.

3:00pm **NT+NS+EM+MS-ThA4 Simulations of Plasticity and Kink Catalyzed Functionalization of C and BN Nanotubes**, ***D. Srivastava,*** NASA Ames Research Center*; M. Menon,* University of Kentucky

Routes to plasticity and kink catalyzed chemistry for functinlaization of C and BN nanotubes are investigated via classical molecular dynamics (MD) and generalized tight-bonding quantum molecular dynamics (QMD) methods. The critical strain for plasticity of BN nanotube is found to be more than that for the similar C nanotube. The structural collapse of nanotubes under compression is explored in which we find that the accumulated strain drives the tube in a plastic deformation in which four-fold coordinated tetrahedral bonds form at the location of the collapse. This lowers the elastic limit of compressed nanotubes to much less than what was predicted earlier with classical MD potential methods alone.@footnote 1@ The critical stress needed for this transition, as computed with QMD method, is in good agreement with experimental values observed for compressed nanotubes in polymer composites and graphite to diamond like transition in a bucky-onion pressure cell. Mechanical kink driven side-wall functionalization of C and BN nanotubes is also explored. We find that mechanical twisting and bending of the tube enhances the binding energy (and lowers the cohesive energy) at kink or edge sites by 1-2 eV as compared to the reactivity of undeformed tubes. Highly localized selective functionalization and etching of sidewalls could thus be possible through kink catalyzed chemical reactivity of nanotubes. A preliminary example of the experimental evidence will be shown.@footnote 2@ @FootnoteText@ @footnote 1@D. Srivastava, M. Menon, and K. Cho, submitted (1999). @footnote 2@D. Srivastava, D. W. Brenner, J. D. Schall, K. D. Ausman, M. F. Yu and R. S. Ruoff, to appear J. Phys. Chem. (1999).

3:20pm **NT+NS+EM+MS-ThA5 Nanoindentation and Nanotribology with Carbon Nanotubes**, *B. Ni, A. Garg,* ***S.B. Sinnott,*** University of Kentucky

The mechanisms by which carbon nanotubule (CNT) proximal probe tips deform during the nanometer-scale indentation and scratching of surfaces are explored using classical molecular dynamics simulations. The forces acting on the atoms in the simulations are calculated using a many-body, reactive bond-order potential for hydrocarbons. The results show that single-walled and multiwalled CNT tips indented against hydrogen-terminated diamond and graphene surfaces buckle and slip to relieve the applied stress. However, in the case of reactive surfaces, tip-surface adhesion occurs on contact that ultimately destroys the tubule. Furthermore, while shell-shell interactions have little effect on the deformation mechanisms, the multiwalled tubule is stiffer than comparably

[1] **Falicov Student Award Finalist**

sized single-walled tubules. Finally, the way in which the deformation of these tubules changes during scratching of diamond and graphene surfaces will be discussed and the results compared to available experimental data. @FootnoteText@ Supported by NASA Ames Research Center (NAG 2-1121) and NSF MRSEC (DMR-9809686).

3:40pm **NT+NS+EM+MS-ThA6 Quantum Chemistry Study of Carbon Nanotube Fluorination**, ***R.L. Jaffe,*** NASA Ames Research Center

Quantum chemistry calculations are carried out to characterize the products of fluorination reactions of C@sub 60@, C@sub 70@ and carbon nanotubes. The calculations utilize density functional theory with a widely used hybrid nonlocal functional (B3LYP-DFT). C@sub 60@ is known to readily undergo reaction with molecular fluorine to form C@sub 60@F@sub n@ with n<44. C@sub 60@F@sub 18@ and C@sub 60@F@sub 36@ are the predominate products. C@sub 70@ also is known to undergo similar reaction, but the products have not been completely characterized. Less is known about the possibility of fluorinating nanotubes. However, it has been conjectured that highly fluorinated nanotubes may have attractive chemical and dielectric properties. Fluorination of C@sub 60@ and C@sub 70@ is used to benchmark the calculations for nanotubes. Previous studies have demonstrated that polycyclic aromatic hydrocarbons with an externally constrained curvature are good model molecules for studying the functionalization reactions of single-walled carbon nanotubes. Reaction is likely if the products are energetically stable and any activation energy barriers are small. Initial studies for C@sub 60@ and (10,10) nanotubes have shown that the difluoronated products are quite stable and the fluorination reaction is highly exothermic.

4:00pm **NT+NS+EM+MS-ThA7 Gear-like Rolling Motion of Carbon Nanotubes on HOPG**, ***M.R. Falvo,*** *J. Steele, A. Buldum,* University of North Carolina, Chapel Hill*; D. Schall,* North Carolina State University*; R.M. Taylor II,* University of North Carolina, Chapel Hill*; D.W. Brenner,* North Carolina State University*; J. Lu, R. Superfine,* University of North Carolina, Chapel Hill

Though much work has been done in recent years in exploring nanometer and atomic scale sliding friction, little experimental or theoretical work has been done on rolling and its relation to sliding at this scale. We will present lateral force microscope investigations of frictional phenomena of multiwall carbon nanotubes (MWCNTs) on highly oriented pyrolytic graphite (HOPG), that include all the rigid body motions: sliding, rotating in-plane, and rolling. Using an advanced manipulation interface for AFMs, the nanoManipulator, we study these friction phenomena through sophisticated manipulation experiments where lateral forces are monitored during manipulations. We have manipulated MWCNTs into a state of atomic registry between the lattice of the tube and underlying substrate. Out of atomic registry the friction is smooth and uniform. As the CNT is rotated in the plane of the substrate, three discrete atomically registered orientations are observed marked by a 3-10 fold increase in the lateral force required to remove them from these orientations. Results of molecular statics calculations for this system show that the potential energy as a function of in-plane rotation angle has three deep minima spaced sixty degrees apart corresponding to atomic lattice registry. When the CNT locks into atomic registry, there is a transition from an in-plane rotational motion to a stick-slip rolling motion. Rather than being perfectly cylindrical, our lateral force data during rolling indicate that the CNT may be faceted (polygonal cross section). MS calculations indicate that faceting is to be expected for MWCNT depending on diameter and wall thickness. The calculated friction expected for rolling a faceted MWCNT agrees well with experimental lateral force data. Molecular dynamics calculations will be shown that lend insight into the energy loss mechanisms for both the sliding and rolling case. This work is supported by the NIH (NCRR), NSF, ONR (MURI), and ARO (DURIP).

4:20pm **NT+NS+EM+MS-ThA8 Selectivity and Diffusion of Binary Fluids in Carbon Nanotubes**, ***Z. Mao,*** *S.B. Sinnott,* University of Kentucky

Carbon nanotube bundles have been proposed as good materials for the manufacture of tailored ultrafiltration membranes due to their uniform, porous structure. In contrast to conventional membranes produced by only partially sintering a ceramic or stretching a polymer, a nanotube membrane would offer the advantages of fewer blocked pores and a narrower distribution of pore sizes. To investigate the properties of a nanotube membrane, the adsorption of simple binary fluids within single tubules and tubule bundles are modeled using atomistic simulations. Specifically, classical molecular dynamics simulations are performed using a combined many-body, reactive bond-order and Lennard-Jones potential. The results show how the diffusion of these molecules proceeds at differing rates within the nanotubes as a function of the diameter and helical structure of the tubules, the density of the fluid, the size difference between the molecules, and temperature. An example of a binary fluid that has been studied is a mixture of CH@sub 4@ and C@sub 4@H@sub 10@ at room temperature. The simulations predict high selectivity in the diffusion of these molecules through the nanotubes. They also allow for the determination of the type of diffusion followed by each type of fluid molecule. Comparisons will be made between these simulation results and the results of similar studies in the literature of diffusion in zeolites and other molecular sieves. @FootnoteText@ Supported by NASA Ames Research Center (NAG 2-1121) and NSF MRSEC (DMR-9809686).

4:40pm **NT+NS+EM+MS-ThA9 Improved Tungsten Disulfide Nanotubes as Tips for Scanning Probe Microscopy**, ***A. Rothschild,*** *G. Frey, M. Homyonfer, M. Rappaport, S.R. Cohen, R. Tenne,* Weizmann Institute of Science, Israel

Synthesis and applications of long and hollow WS@sub 2@ nanotubes are described. Although synthesis of nanotubes from various inorganic compounds have been reported, the high yields of uncontaminated nanotubes reported here represents a significant improvement over past efforts by ourselves and others.@footnote 1@,@footnote 2@ The nanotubes are synthesized in a two-step process the first being the creation of WO@sub 3@ nanoparticles by heating a tungsten filament in the controlled presence of water. The second step, sulfidization, resulted in a 30 times increase in the length of these particles without change in width so that nanotubes up to 10 microns in length and 20-40 nm width were formed. These tubes were attached to scanning force microscope (SFM) tips and used to image deep and sharp features inaccessible by sharp silicon tips. Due to their sandwich S-W-S structure, these nanotubes are probably stiffer than the carbon analogs and hence less prone to instabilities under such rigorous scanning conditions. We propose application of these probes for nanophotolithography, aided by the facile excitation of these compounds by visible and infra-red light. Support by the Israel Ministry of Science, Israel Science Foundation, and Applied Materials-Weizmann Foundation are gratefully acknowledged. A.R. is a recipient of the Lavoisier fellowship (France). @FootnoteText@ @footnote 1@ Y. Feldman, E. Wasserman, D.J. Srolovitz, R. Tenne, Science 267, 222 (1995). @footnote 2@ N.G. Chopra, et al, Science 269, 966 (1995).

Surface Science Division
Room 606 - Session SS1+EM+NS-ThA

Metal/Metal Growth

Moderator: R.Q. Hwang, Sandia National Laboratories

2:00pm **SS1+EM+NS-ThA1 Dislocation Structures of Submonolayer Films near the Commensurate-Incommensurate Phase Transition: Ag on Pt(111)**, ***J.C. Hamilton,*** *R. Stumpf,* Sandia National Laboratories*; K. Bromann, M. Giovannini, K. Kern, H. Brune,* EPF Lausaane, Switzerland

We provide a theoretical explanation@footnote 1@ for unusual experimental observations@footnote 2@ of submonolayer Ag film growth on Pt(111). These films exhibit parallel partial dislocations with narrow hcp regions separated by much wider fcc domains. Using a 2D Frenkel-Kontorova (FK) model we show that this unusually large difference is primarily due to proximity to the commensurate-incommensurate phase transition, and only secondarily to stacking fault energies. We next consider the relationship between island energy, island dislocation structure, and island shape. Using the FK model we calculate the stability of islands with no dislocations, a single dislocation pair across the island, two parallel dislocation pairs across the island, and a "Y" shaped dislocation structure. The model is in excellent agreement with experiment in predicting the onset of dislocation structures in growing islands. It also suggests that the dislocations have little or no effect on the equilibrium island shape. Finally we discuss the relationship between these calculations and related experiments@footnote 3@ on the structure of the clean Pt(111) surface which reconstructs above 65% of the melting point. @FootnoteText@ @footnote 1@ J. C. Hamilton, R. Stumpf, Karsten Bromann, Marcella Giovannini, Klaus Kern and Harald Brune, Phys. Rev. Lett., in press@footnote 2@ Karsten Bromann, Harald Brune, Marcella Giovannini, and Klaus Kern, Surf. Sci. V388, L1107 (1997). @footnote 3@ A. R. Sandy, S.G.J. Mochrie, D.M. Zehner, G. Grubel, K.G. Huang and Doon Gibbs, Phys. Rev. Lett. 68, 2192 (1992).

2:20pm **SS1+EM+NS-ThA2 Non Capillarity Driven Grain Growth in a Strained Cu Ultrathin Film**, ***A.K. Schmid***, *T. Giessel, N.C. Bartelt, J. de la Figuera, R.Q. Hwang,* Sandia National Laboratories

Properties of metal films are crucially influenced by details of their grain structure. To determine basic mechanisms of grain evolution we have investigated a prototypical granular thin film using LEEM and STM. In two monolayer thick films of Cu on Ru(0001) a uniaxial relaxation relieves the misfit strain (5.5%) with the substrate, leading to a two-dimensional grain structure consisting of three orientationally different domain types. We observed in-situ grain growth using LEEM in dark field imaging mode and took STM snap shots at several stages of the grain evolution. While on large scale of both time and area the total length of grain boundary decreases in order to reduce the free energy of the system an increase of boundary length has been observed locally and on smaller time scale. The observed behavior can not be described within the framework of a Q-state Potts model which has been widely used for the description of grain growth. We show that the long-ranged lateral interactions between the surface atoms in the strained Cu film which are not considered in Potts model are responsible for the observed behavior.

2:40pm **SS1+EM+NS-ThA3 Exchange Processes in Metal on Metal Growth Studied with High-resolution STM**, ***M. Schmid,*** Technische Universitaet Wien, Austria **INVITED**

In the early 1990's, after the first atomic-scale studies by field ion microscopy and related simulation calculations it became apparent that many processes in growth of thin films involve exchange of substrate and deposited atoms. It was concluded that interlayer diffusion at steps, the key process determining the growth mode, often occurs by replacing a substrate atom with a deposited atom, pushing the substrate atom onto the lower terrace. A new way to study such phenomena is scanning tunneling microscopy (STM) with atomic resolution and chemical contrast@footnote 1@. We have deposited a small amount of Co on a Pt(111) surface with a high density of steps. In the resulting structure, we can distinguish between substrate (Pt) and deposited material (Co) on an atom-by-atom basis. An analysis of the STM data shows that Co atoms do not descend Pt steps by diffusing over the step, but descend from the upper terrace to the lower by an exchange diffusion process at the step edge with the Pt atoms. The Co atoms descend a Pt step edge by this process neither at straight A nor at B steps, but rather at the corners or kinks of the vacancy islands. These results are in qualitative agreement with simulations based on embedded atom method (EAM) potentials. Other examples of exchange processes can lead to subsurface growth of the deposited material, with substrate atoms floating on top of it. Such phenomena were observed to occur already at or near room temperature when Co was deposited on the Pt(111) and Pt(110) surfaces. @FootnoteText@ @footnote 1@ E. Lundgren, B. Stanka, G. Leonardelli, M. Schmid, and P. Varga, Phys. Rev. Lett., accepted.

3:20pm **SS1+EM+NS-ThA5 Self-diffusion on Pt(110)-1x2: Ab-initio Barriers vs. Experiment@footnote 1@**, ***P.J. Feibelman,*** Sandia National Laboratories

Because it requires breaking more bonds, dimer diffusion by dissociation and recombination on clean Pt(110)-1x2 should cost more energy than the recently discovered@footnote 2@ "leapfrog" mechanism. Since cohesion per bond decreases with increasing coordination, the leapfrog mode should also have a lower barrier than monomer diffusion. Though first-principles calculations confirm these deductions, they are at odds with experiment, possibly signalling the influence of low-level surface contamination. @FootnoteText@ @footnote 1@ Work supported by the U. S. Department of Energy under Contract No. DE-AC04-94AL85000. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy @footnote 2@ T.R. Linderoth, et al., Phys. Rev. Lett. 82, 1494(1999); F. Montalenti and R. Ferrando, Phys. Rev. Lett. 82, 1498(1999).

3:40pm **SS1+EM+NS-ThA6 Novel Temperature Dependence of the Morphology of Deposited Multilayer Ag/Ag(100) Films**, ***C.R. Stoldt,*** *A.R. Layson, C.J. Jenks,* Iowa State University*; M.C. Bartelt,* Sandia National Laboratories*; K. Caspersen, J.W. Evans, P.A. Thiel,* Iowa State University

Metal(100) homoepitaxy provides a natural testing ground for recently developed ideas on kinetic roughening and "mound formation" due to step-edge barriers. Non-monotonic variation of roughness with deposition temperature (T) has been predicted,@footnote 1@ but not observed. Here, we report comprehensive VT-STM studies for growth of Ag/Ag(100) films between 130K and 300K which reveal this behavior. Roughness of 25ML Ag/Ag(100) films at first increases "classically" below 300K due to inhibited downward transport, but then decreases below 220K, achieving a low plateau value below 170K. Unlike Pt/Pt(111) and Rh/Rh(111) growth, non-monotonic behavior is not associated with a dramatic change in 2D island morphology, but rather with enhanced downward funneling from (the more prevalent) step edges at lower T. We also characterize the mound morphology, noting the steepness of the mound sides and small lateral dimension at lower T. A breakdown of kinematic scattering behavior of the intensities observed in our HRLEED studies of these films is attributed to this feature. Monte Carlo simulations of a realistic model for growth@footnote 1@ are consistent with and elucidate observed behavior. @FootnoteText@ @footnote 1@M.C. Bartelt and J.W. Evans, Surf. Sci. 423 (98) 189; Phys. Rev. Lett. 75 (95) 4250.

4:00pm **SS1+EM+NS-ThA7 Edge Diffusion During Growth: Kink Ehrlich-Schwoebel Effect and Resulting Instabilities@footnote 1@**, *O. Pierre-Louis,* Univ. J. Fourier (CNRS), France*; **T.L. Einstein,*** University of Maryland

In addition to the usual step Ehrlich-Schwoebel effect (SESE) on typical metal and semiconductor surfaces, there can also be a kink Ehrlich-Schwoebel effect (KESE), associated with asymmetries in barriers at kinks/corners encountered by atoms during transport along step edges.@footnote 2@ We take into account both phenomena to study the evolution of arbitrarily oriented surfaces during molecular beam epitaxy. We find that the heretofore rarely discussed@footnote 3@ KESE has a profound effect on growth morphology. Under the usual growth conditions, KESE induces a new instability of vicinal surfaces, supplanting the familiar Bales-Zangwill instability@footnote 4@ due exclusively to SESE. The possibility of stable kink flow growth is analyzed; fluctuations can shift the stability threshold. For some orientations, KESE can stabilize steps. KESE can also induce mound formation. @FootnoteText@ @footnote 1@Work supported by NSF MRSEC grant DMR 96-32521. @footnote 2@ O. Pierre-Louis, M. R. D'Orsogna, and T. L. Einstein, Phys. Rev. Lett. 82 (1999) 3661; note also M. V. Ramana Murty and B. H. Cooper, preprint. @footnote 3@ See, however, I. L. Aleiner and R. A. Suris, Sov. Phys. Solid State 34 (1992) 809; Z. Zhang and M. G. Lagally, Science 276 (1997) 377; J. G. Amar, Bull. Am. Phys. Soc. 43 (1998) 851 and to be published. @footnote 4@ G.S. Bales and A. Zangwill, Phys. Rev. B 41 (1990) 5500.

4:20pm **SS1+EM+NS-ThA8 Atom-by-Atom Growth: Bonding and Rebonding on Metal Surfaces**, ***A. Bogicevic,*** Sandia National Laboratories

The bond-order--bond-length concept put forth by Pauling almost 70 years ago has greatly added to our intuitive understanding of atomic-scale bonding in molecules. The basic idea is that the more bonds an atom makes, the weaker and longer each becomes [rebonding]. This concept has been extensively tested, and is routinely used in molecular chemistry today, so one would assume that a similar model for the gas-surface interface would prove useful. In an early first-principles study of Al/Al(100), strong and observable rebonding effects were predicted. Unfortunately, these results are an artifact of some severe modelling compromises imposed by computational limitations. New, fully converged (160-180 atom unit-cells, 36 k-points), first-principles density-functional calculations for a wide variety of homogeneous and heterogeneous metal systems show that, contrary to rebonding theory, addimers (adsorbed atom pairs) do not have longer surface bonds than adatoms, do not reside farther above the surface, and do not meet the rebonding arguments for augmented mobility. Rebonding does contribute to destabilize addimers, but does not explain inherently weak adatom-adatom interactions. I explain the absence of rebonding effects in terms of elastic and electronic contributions to the rebonding energy, and present an alternative explanation for the adatom-adatom bond weakness based on bond frustration. Implications for nucleation and growth of metals will be discussed.@footnote 1@ @FootnoteText@ @footnote 1@ Work at Sandia National Laboratories is supported by the U.S. Department of Energy under Contract DE-AC04-94AL85000. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy.

4:40pm **SS1+EM+NS-ThA9 Diffusion of Lead on the Au(111) Surface Studied by Scanning Tunneling Microscopy and Embedded-Atom Method Molecular Dynamics**, ***M.C. Robinson,*** Trent University and Queen's University, Canada*; K. De'Bell,* University of New Brunswick in Saint John, Canada*; A.J. Slavin,* Trent University and Queen's University, Canada

Low coverages of Pb deposited on the reconstructed Au(111) surface have been studied with STM and show that the reconstruction strongly influences diffusion and film morphology. Nucleation sites for Pb adatoms are found at the kinks of the reconstruction. For higher coverages, Pb atoms concentrate in the fcc and hcp regions; the elevated transition

regions are much less populated. The reconstruction is lifted for some coverage between 0.05 and 0.3 monolayers (ML). For comparison, the Embedded Atom Method-Molecular Dynamics (EAM-MD) method has been used to study diffusion of Pb on both the unreconstructed (flat) and reconstructed surfaces. EAM-MD simulations show that diffusion is complicated by the reconstruction. Using both static and dynamic methods, the diffusion energies have been determined. They show that, for an adatom moving perpendicular to the compression direction, the energy barrier is 1.7 times greater than for motion in the parallel direction. Diffusion is slowed on the fcc part of the reconstructed surface, as compared to the unreconstructed, by a factor of about 2. No greater coverage than 0.07 ML could be forced onto the EAM-modelled reconstructed surface. However, the flat surface could be fully covered, suggesting that the reconstruction is not energetically stable at higher coverages, as has been observed experimentally.

5:00pm **SS1+EM+NS-ThA10 Low Energy Electron Microscope Investigation of Pb Overlayers on Cu(100)***, **G.L. Kellogg**,* Sandia National Laboratories

Pb overlayers on Cu substrates provide a model system for investigating epitaxial films exhibiting large lattice misfits and for studying two-dimensional phase transitions (e.g., disordering and surface melting). On Cu(100), room-temperature deposition of Pb follows classical Stranski-Krastanov growth with three well-defined overlayer structures forming at submonolayer coverages.@footnote 1@ In this investigation, low energy electron microscopy (LEEM) is used to (1) characterize the changes that occur to these structures resulting from annealing to various temperatures and (2) monitor the subsequent growth of 3-D islands. The low-coverage c(4x4) and high-coverage c(5@sr@2x@sr@2)R45 phases, both of which consist of rotationally inequivalent domains, are observed to disorder at temperatures of 270C and 215C, respectively. By forming images using selected low energy electron diffraction beams (i.e., dark-field LEEM), the domain structure that forms upon cooling from above the transition temperature is imaged directly with a spatial resolution of ~10 nm. Dark-field LEEM is also used to characterize the c(4x4) - c(2x2) co-existence structure that forms upon desorption of excess Pb from the high-coverage phase. The growth of three-dimensional Pb islands on top of the high-coverage phase and the coarsening of these structures at temperatures from 100-150C are measured to derive fundamental energetic parameters involved in the melting of 3-D Pb clusters. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U. S. DOE under Contract DE-AC04-94AL85000 @FootnoteText@ @footnote 1@ J. Henrion and G. E. Rhead, Surface Sci. 29(1972)20.

Nanometer-scale Science and Technology Division
Room 611 - Session MS+PS-FrM

Diagnostics and Processes in Etching

Moderator: P.L.G. Ventzek, Motorola Inc.

8:20am **MS+PS-FrM1 Effect of CH@sub 3@F/C@sub 4@F@sub 8@ Ratio on the SiO@sub 2@-to-Si@sub 3@N@sub 4@ Selectivity in a Self-Aligned-Contact Etching Process for Giga-bit DRAM**, ***S.C. Park,*** Hyundai Electronics Industries Co. Ltd., Korea*; J.S. Kim,* Hyundai Electronics Industries Co. Ltd., Korea, South Korea*; J.J. Lee, K.T. Kim, D.D. Lee, Y.S. Seol, I.H. Choi,* Hyundai Electronics Industries Co. Ltd., Korea

Effect of CH@sub 3@F/C@sub 4@F@sub 8@ ratio on the SiO@sub 2@-to-Si@sub 3@N@sub 4@ selectivity in a self-aligned-contact(SAC) oxide etching process was investigated using an inductively coupled plasma. As published in other studies, the SiO@sub 2@-to-Si@sub 3@N@sub 4@ selectivity usually increases as the CH@sub 3@F/C@sub 4@F@sub 8@ ratio increases.@footnote 1@ However, we found out in this work that the selectivity gradually increases to a specific peak and sharply drops as the CH@sub 3@F/C@sub 4@F@sub 8@ ratio continuously increases. Moreover, the selectivity was extremely poor at the valleys between the word lines (and in some cases, the nitride layer was even 'punched through'), while the selectivity was very high at the top shoulder of word line at a certain CH@sub 3@F/C@sub 4@F@sub 8@ ratio. It was found from the XPS and SEM analysis that the fluorocarbon film was built up without any bonding state change, as the CH@sub 3@F/C@sub 4@F@sub 8@ ratio increased. The increase in the selectivity with increasing CH@sub 3@F/C@sub 4@F@sub 8@ ratio should be related with the amount of the fluorocarbon polymer deposition on the surface of Si@sub 3@N@sub 4@ barrier.@footnote 2@ However, the analysis of the fluorocarbon films could not completely explain the sharp drop in the selectivity and the extremely low selectivity at the valley between the word lines. Further studies showed that step coverage of the polymer film formed during the SAC oxide etching was very poor as the contact size decreased and the CH@sub 3@F/C@sub 4@F@sub 8@ ratio increased. In this case, less amount of the fluorocarbon gases should enter the contact hole and less amount of fluorocarbon polymer should be deposited on the Si@sub 3@N@sub 4@ etch barrier. This will eventually result in the sudden drop in the selectivity. @FootnoteText@ @footnote 1@ Y. Iijima and H. Okano, Jpn. J. Appl. Phys, Vol. 36, 5498 (1997) @footnote 2@ N.R. Rueger and G.S. Oehrlein, J. Vac. Sci. Technol. A 15, 1881 (1997

8:40am **MS+PS-FrM2 Plasma Cleaning of Via Bottoms Following Dielectric Etching**, ***P.J. Matsuo,*** *M. Schaepkens, G.S. Oehrlein,* State University of New York at Albany

In plasma etching, aspect ratio effects have been well documented. However,the dependence of the necessary cleaning steps following the etch on feature geometry have not. Cleaning via bottoms following the dielectric etch step can be critical to achieving low resistance contacts in multi-layer metallization schemes. Reducing this resistance is a prerequisite for the proper electrical function of Cu/low-k dielectric wiring architecture. We have examined in-situ surface modifications of post-etch blanket surfaces of several materials (Si, Cu, TiN, Al), resulting from Ar and O@sub 2@ cleaning treatments, using ellipsometry and XPS. We also investigated the removal efficiency of fluorocarbon and oxide residues at via bottoms for realistic aspect ratio structures by measuring the removal rate of fluorocarbon films or oxide films during O@sub 2@ plasma and Ar sputter cleaning, respectively. Ion driven cleaning procedures such as oxide removal, do not show a significant dependence on feature aspect ratio. On blanket films, to vias with an aspect ratio of 3, Ar sputter rates of BPSG remain constant. The removal of fluorocarbon residues under high density O@sub 2@ plasma exposure is heavily dependent on the neutral flux and is reduced in accordance with geometrical shadowing offset by the constant ion component. We have also investigated the surface chemistry of the residues as a function of feature geometry and cleaning process parameters.

9:00am **MS+PS-FrM3 Molecular Dynamics Simulations of Fluorocarbon Films**, ***J. Tanaka,*** Hitachi, Ltd., Japan*; C.F. Abrams, D.B. Graves,* University of California, Berkeley

Fluorocarbon plasma processes are used for highly selective etch processes of SiO@sub 2@ with respect to Si, SiN or photoresist. During fluorocarbon plasma etching, it is known that fluorocarbon films form on the latter surfaces, protecting them from active etch species such as F atoms. Even on actively etched surfaces of SiO@sub 2@, thin fluorocarbon films have been detected. During etching, the fluorocarbon films are an active participant, and in order to optimize etch processes, understanding these films is important. However, the structure and mechanisms of fluorocarbon film formation are not well understood. The nature of fluorocarbon film structure and its role in etching depend on the neutral and ionic species that impact it from the plasma, as well as the underlying material. We have chosen to use molecular dynamics of fluorocarbon ions impacting a carbon surface as a first step in understanding this complex process. In order to use molecular dynamics, we have developed a new C-F intermolecular potential. Our potential was developed based on the reactive empirical bond order (REBO) potential, using a strategy originally developed for carbon-hydrogen interactions. (Brenner, Phys. Rev. B, Vol.42, pp.9458) Initially, we calculated the argon ion sputtering yield of carbon at 100eV, 300eV and 500eV. For this low energy region, TRIM simulator significantly underestimated the sputtering yields while the yields calculated by the MD simulation agreed well with experimental results. Next, we simulated CF, CF@sub 2@, and CF@sub 3@ ion impacts at 100eV and normal incidence onto an amorphous carbon surface. In all cases, the initial process was net fluorocarbon film deposition at low fluences. For CF@sub 2@ and CF@sub 3@ ions, the fluorocarbon film reached a steady state thickness after several hundred ion impacts. In this talk, we will present the simulated film composition profile and the species that chemically and physically sputter from the surface as a function of ion fluence for each of the three ions simulated. In addition, the angular dependence of both film composition profile and sputtering characteristics will be presented.

9:20am **MS+PS-FrM4 Plasma-Induced Roughening of Resist**, ***S. Halle,*** *W.H. Yan, W. Moreau,* IBM Microelectronics*; J. Wittmann, A. Gutmann,* Infineon Technologies

A severe etch-induced line edge roughness of the resist pattern transfer during dielectric mask open reactive ion plasma processes is increasingly becoming a major issue in semiconductor processing as resist stacks shrink below 700 nm with sub 200 nm lithography. The resulting patterned features are observed to have serrated or "scallop-like" sidewall surfaces which are typically translated from the remaining resist / ARC layer to the dielectric layers and into the silicon, in both device contact-type and active area line space features. The origin of this effect, which results in a roughening of the silicon sidewalls and may severely compromise the patterned feature integrity, is poorly understood. In this study, we show that etch process conditions which produce "scallop-like" distortions are associated with a high degree of resist surface roughness as observed by SEM and measured by AFM. The roughening of a blanket resist surface exposed to reactive ion plasma etching is associated with a large "grain" size in the xy plane and a high "pitting" frequency in the z (depth) axis. The pitting frequency on blanket wafers is found to be qualitatively equivalent to the line edge roughness on patterned features. The extent of roughness is found to be highly sensitive to changes in etch process conditions such as bias voltage, chamber pressure, and gas flow constituents. The resist surface roughness, is examined under the following process conditions: argon sputtering only, fluorocarbon etching with low polymerization, fluorocarbon etching with a higher degree of polymerization. The contribution of the sputter component is found to be dominant; however, polymerizing fluorocarbon chemistry can also modulate the roughness. A qualitative model to explain the formation of the "scallop-like" features will be discussed.

9:40am **MS+PS-FrM5 Measurement of Residual Fluorine in a Polysilicon Etch Reactor with Fourier Transform Infrared Spectroscopy (FTIR)**, ***J.E. Daugherty,*** *E. Edelberg, V. Vahedi, A. Perry, J. Huang, R. Marsh,* Lam Research Corporation

One challenge in sub-0.18 µm gate etching is maintaining the integrity of the thin (<25 Å) gate oxide. This task is especially difficult for in situ hardmask applications where a dielectric (SiO@sub 2@ or Si@sub 3@N@sub 4@) hardmask is etched with a fluorine-containing gas (e.g., CF@sub 4@) in the same chamber that the underlying polysilicon gate is etched with Cl@sub 2@ and HBr. Fluorinated molecules can be released from in-chamber etch residues for several minutes after the fluorine-containing etchant is turned off, and free fluorine is produced when the plasma subsequently dissociates these compounds. If there is sufficient fluorine remaining in the chamber after the polysilicon is etched, it can reduce the selectivity to the underlying gate oxide. A similar reduction of the gate oxide selectivity is often noticed immediately following a dry clean of the etching chamber (i.e., a plasma clean). Since the chamber is cleaned with SF@sub 6@ or NF@sub 3@ plasma, residual fluorine from the cleaning plasma sometimes reduces the amount of remaining gate oxide

on the first wafer processed after the clean. We have used Fourier transform infrared spectroscopy (FTIR) to measure the concentration of several fluorine-containing etch products (e.g., SiF@sub 4@, HF) during gate etching with Cl@sub 2@/HBr in an inductively coupled plasma reactor. We have verified that the etch rate of thermal SiO@sub 2@ in Cl@sub 2@/HBr mixtures increases with increasing concentration of residual fluorinated etch products in the effluent of the reactor. We also observe that for in situ hardmask etching, the amount of fluorine-containing etch product that is observed at the end of the polysilicon etch step depends on the duration of fluorine exposure during the hardmask etch step.

10:00am **MS+PS-FrM6 Effect of W Reaction Byproducts on W/poly-Si Stack Gate Etching Process**, ***H. Morioka***, *M. Nakaishi, N. Abe,* Fujitsu Limited, Japan

W/(barrier layer)/poly Si stack is one of the most promising candidate for gate electrode structure of memory-embedded logic LSIs and DRAMs in the next generation because of low sheet resistance and compatibility with self-aligned contact (SAC) process, etc. Generally, the chemistry of W/poly Si stack gate etching is halogen-base, and most of W etching chemistry have higher etch rate of poly-Si than that of W itself. Although oxygen addition can increase the selectivity to poly Si above 1 by inhibiting Si etching, some troubles are still observed during poly Si etching step, such as non-uniform enhancement of etch rate, undercut profile, and serious RIE-lag. These facts make it difficult to achieve W/poly Si stack gate etching against very thin gate oxide. So, we examined the effect of W reaction byproducts on etching characteristics of other layers. Our experiments were performed on a high-density plasma (HDP) etcher whose plasma source could be operated in continuous mode or pulse modulated mode. We also compared fluorine-base chemistry with chlorine-base one to investigate the difference of etching byproducts. In this experiment, we found that W etching byproducts from a sample wafer and chamber wall enhanced the etch rate of poly-Si and SiO@sub 2@ especially for chlorine-base chemistry, and pulse modulation of plasma could reduce this enhancement. These facts suggest that W etching byproducts were decomposed into fragments in the plasma, these species were deposited on the sample surface and varied the etching characteristics. It is probable that pulse modulation reduced the dissociation of W reaction byproducts because of low electron temperature during afterglow.

10:20am **MS+PS-FrM7 Vacuum- and Near-Ultraviolet Spectra of Plasma Etching Discharges**, ***J.R. Woodworth***, *T.W. Hamilton, B.P. Aragon,* Sandia National Laboratories

We are measuring the absolute intensities of the Vacuum- and Near- UV emission spectra (24 eV to 4 eV) in metal etch and oxide etch plasmas in an inductively-driven Gaseous Electronics Conference reference cell. These spectra are of interest both because UV radiation may damage the circuits being processed and changes in the spectra may be used for process control. Spectra are being taken both in a cell with stainless steel electrodes and in a cell whose electrodes are covered with aluminum oxide, quartz and silicon to better simulate a commercial etch tool. In metal etch discharges containing mixtures of Cl2, BCl3, Ar, and N2, the vacuum ultraviolet spectrum above 8.8 eV is dominated by atomic Cl lines and Ar lines between 9 and 12 eV. Very little energy is emitted between 12 and 24 eV. The near ultraviolet spectra from 8.8 to 4 eV are dominated by B, BCl, Cl2, and etch products such as Si. Details of the experiments, effects of biasing the wafer, absolute line intensities and the effect of radiation trapping on the discharges will be discussed. This work was supported by the United States Department of Energy under Contract DE-AC04-94-AL85000. Sandia is a multiprogram laboratory operated by the Sandia Corporation, a Lockheed Martin Company, for the United States Government

10:40am **MS+PS-FrM8 Etching of Organic Low Dielectric Constant Materials on the Lam Research 4520XLE**, *C. Janowiak,* ***S.L. Ellingboe***, *J. Flanner, I. Morey,* Lam Research Corporation

The low dielectric constant (k) of the polymeric materials SiLK and BCB have made them an attractive possible alternative to silicon dioxide as an intermetal dielectric in IC circuits. The lower dielectric constant is desirable to reduce capacitance and RC delay for higher chip speed, less cross talk, and lower power consumption. The forming of via and trench patterns in these low-k materials using a dry etch chemistry was investigated. Because SiLK and BCB is a polymeric material, oxygen is used as the primary etch gas, nitrogen as a dilulent and a hydrocarbon for sidewall passivation. Typically the organic low-k etch has a selectivity of low-k:PR ~1:1. Depending on the film structure, the PR can clear during the low-k etch, exposing the oxide hardmask for the latter portion of the etch. In the 4520XLE, this corresponds to a change in the etch process from a chemically dominated etch to an ion-dominated etch. Consequently, the plasma chemistry changes upon PR clearing and TEOS exposure, which can result in changes to etch rate, etch rate uniformity, and etch rate profile. Simulations of the SiLK etch results will be shown along with process results. The effects of process parameters such as RF power and oxygen-hydrocarbon ratio on etch performance will be discussed.

Topical Conference on Emerging Opportunities and Issues in Nanotubes and Nanoelectronics

Room 6C - Session NT+NS+EM+MS-FrM

Nanotubes: Growth, Characterization and Properties II

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

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

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

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

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

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

The electronic and electrochemical properties of Li intercalated single-wall nanotube ropes are studied theoretically using ab initio method@footnote 1@ and experimentally in an electrochemical cell.@footnote 2@ Complete

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

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

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

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

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

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

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

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

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

Author Index

Bold page numbers indicate presenter

Author Index

Author Index