

Monday Morning, October 31, 2011

Electron Transport in Low Dimensional Materials Focus

Topic

Room: 209 - Session ET+EM+SS-MoM

Quantum Transport: From 0- to 2-Dimensions

Moderator: A.-P. Li, Oak Ridge National Laboratory, K. Varga, Vanderbilt University

8:20am **ET+EM+SS-MoM1 Charge and Spin Transports at Surfaces of Strong Spin-Orbit-Coupling Materials.** *S. Hasegawa, T. Hirahara*, University of Tokyo, Japan **INVITED**

Transports of charge as well as spin at crystal surfaces are now intensively studied by various kinds of experiments. Surface electronic states are generally decoupled from the bulk states and therefore intrinsically low-dimensional. Furthermore, space-inversion symmetry is broken down at crystal surfaces; one side of the surface is empty vacuum while other side is full of electrons in the crystal. These effects provide rich physics of transport, especially on surfaces of strong spin-orbit-coupling (SOC) materials. The surface-state bands are known to be spin-split of such strong SOC crystals such as Bi and Bi alloys, which is called by Rashba effect [1-4]. Similar effect is observed on a special kind of materials called topological insulators such as BiSb, BiSe, and BiTe alloys. Some of them have spin-split Dirac-cone type surface-state bands. This implies that spin-polarized current will flow at the surfaces of such materials.

In my presentation, by using samples of pure Bi [1-4], BiSb [5], BiSe [6,7], and BiTe, I will show that the surface-state bands are really spin-split and the Dirac-cone conductivity is directly measured by microscopic four-point probe method. An on-going project to detect the spin-polarization of surface current by using magnetic tips in a four-tip STM will be also introduced.

[1] T. Hirahara, et al., Phys. Rev. Lett. 97, 146803 (2006).

[2] T. Hirahara, et al., Phys. Rev. B 76, 153305 (2007).

[3] T. Hirahara, et al., Appl. Phys. Lett. 91, 202106 (2007).

[4] T. Hirahara, et al., New J. Phys. 10, 083038 (2008).

[5] T. Hirahara, et al., Phys. Rev. B81, 165422 (2010).

[6] Y. Sakamoto, et al., Phys. Rev. B81, 165432 (2010).

[7] T. Hirahara, et al., Phys. Rev. B82, 155309 (2010).

9:00am **ET+EM+SS-MoM3 Electron Transport in Ferroelectric Domains and Walls.** *A. Baddorf*, Oak Ridge National Laboratory **INVITED**

Ferroelectric tunneling, where electron transport is controlled by the polarization state, has recently been realized in a number of experiments. Polarization-controlled transport effects have been detected in tunnel junctions, thin films, single crystals and at domain walls. Yet, little analysis of data has undertaken to determine the transport mechanisms and their interaction with ferroelectric fields and domain boundaries involved in switching. We present seminal experimental observations of transport in thin films of $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$ (PZT) and BiFeO_3 (BFO). Earlier we have shown that both materials exhibit pronounced polarization-controlled electroresistance [1]. Temperature and voltage dependence of currents are not well fit by any one standard model. Instead a transition between surface and bulk limiting effects is observed. Upon close inspection, I-V curves exhibit a reproducible region of negative differential conductance associated with ferroelectric switching. Although this anomaly may originate from extrinsic processes, e.g. due to oxygen vacancies or charge injection, we have carried out a series of control experiments on PZT films that unequivocally connect variation of conductance with the size of the polarization domain in the plane of the surface. The I-V anomaly therefore originates from significant conductivity of the domain wall and a relatively slow expansion of the domain following polarization switching. However, our results do not imply simply that transport is through domain walls, but further that nanoscale domains formed by switching have fundamentally different conduction behavior [2]. We suggest that domains formed by tip-applied bias have curved walls and are consequently charged, modifying adjacent material much as charge accumulation modifies a semiconductor. Engineering the ferroelectric domain size produces a tunable conductance reminiscent of analogue memristors, providing a quasi-continuous spectrum of non-volatile resistive states, even though the PZT polarization itself is bistable. Ferroic memristive behavior, which based on our measurements is likely to be universal to ferroic semiconductors, is a striking departure from the conventional picture of discrete electron transport states in ferroelectrics.

Research was conducted at the Center for Nanophase Materials Sciences and sponsored by the Division of Scientific User Facilities, U.S. Department of Energy.

[1] P. Maksymovych et al., Science 324 (1421) 2009.

[2] P. Maksymovych et al., submitted.

9:40am **ET+EM+SS-MoM5 Electronic Instabilities, Fluctuations, and Transport in Epitaxial Nanowires.** *H.H. Weitering*, University of Tennessee and Oak Ridge National Laboratory **INVITED**

Quantum transport is at the heart of nanoscience and marries a fundamental law of nature — quantum mechanics — with applied electrical engineering and emerging materials technologies. Ultimately, nanoscale electronic devices will contain networks of wires whose cross sections will be so small as to represent one-dimensional conductors with novel transport properties. We have fabricated exceptionally long and uniform YSi_2 nanowires via self-assembly of yttrium atoms on Si(001). The wire widths are quantized in odd multiples of the Si substrate lattice constant. The thinnest wires represent one of the closest realizations of the isolated Peierls chain, exhibiting van Hove type singularities in the one-dimensional density of states and charge order fluctuations below 150 K. Conduction through individual nanowires follows an inverse Arrhenius behavior, indicative of thermally-assisted tunneling of small polarons between defect centers. Quantitative analysis of individual wire resistances, probe resistances, and negative differential resistances of nanowire networks indicates significant electronic interwire coupling below 150 K. The long-range coupling mechanism involves the dielectric polarization of the substrate, which induces current blockades in neighboring conduction channels.

This work is sponsored by the NIH/NHGRI and was partially conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy

10:40am **ET+EM+SS-MoM8 Grain Boundary Resistivity in Copper Nanowires.** *T.H. Kim*, POSTECH, South Korea **INVITED**

The reliable choice of the interconnect materials in current integrated circuits is copper because of its higher electrical conductivity and improved stability against electromigration among all possible candidates. However, as the width of interconnects is approaching a mean free path of the electrons, the resistivity of copper interconnects is known to increase dramatically. Typically, this increase in the resistivity of the narrow interconnect is attributed to enhanced sequential scattering of electrons from defect planes such as either grain boundaries (GB) or other surfaces/interfaces. But, it is very challenging to distinguish which scattering factor is dominant over others in such a small scale.

To answer such a fundamental question, theorists developed semi-empirical methods and the relative contribution of various electron scattering mechanisms has been understood largely by relying on the semi-empirical methods based on the theories of Fuchs-Sondheimer and Mayadas-Shatzkes. The direct measurements of the resistance of individual GBs have been surprisingly lacking mainly due to technical difficulty to access single GBs in a nanowire that could not be realized by conventional fabrication methods using a fixed electrical contacts. Recently, Y. Kitaoka *et al.* have observed a resistance change along a damascene Cu interconnect wire with four-probe scanning microscope. They successfully separated the GB scattering effect from other scattering sources; however, the direct correlation between the GB structure and the specific GB resistivity remained unclear.

Here we present the direct measurement of individual GB resistances and the critical role of GB structure in the increased resistivity in copper nanowires with a four-probe scanning tunneling microscope. The resistances of high symmetry coincidence GBs are then calculated using a first-principle method, which confirms that the coincidence GBs have orders of magnitude smaller resistance than those measured at the high-angle random GBs. As well, to explain high resistivity of random GBs, we used free-electron-with-random-point-scatterer (FERPS) model. In the FERPS model, we derived that the specific GB resistivity of random GB is independent of the specific structures of random GB such as orientation and is determined entirely by the Fermi wavelength of the bulk.

This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

11:20am **ET+EM+SS-MoM10 Tunable Coulomb Blockade and Giant Coulomb Blockade Magnetoresistance in a Double Quantum Dot System**, *X.-G. Zhang*, Oak Ridge National Laboratory, *T. Xiang*, Chinese Academy of Sciences

We propose a Hubbard model to describe the tunneling effect of electrons in a double quantum dot system connected in the parallel circuit configuration to electrodes. The change in the interdot coupling is shown to dramatically influence the Coulomb blockade properties. For magnetic double dots, the interdot coupling can be tuned by the external magnetic field, leading to a giant Coulomb blockade magnetoresistance. Possible detection of this effect in organic systems is discussed.

This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

11:40am **ET+EM+SS-MoM11 Quantum Transport in Crossbar Devices**, *B. Cook*, *P. Dignard*, *K. Varga*, Vanderbilt University

Electronic devices with crossbar geometries have recently been fabricated with nanoscale features (Zhong, et al, Science Vol. 302). Consisting of a two dimensional grid, devices have been formed with a variety of components including carbon nanotubes and semiconductor nanowires. These devices are assumed to operate classically, but as the dimensions of the device shrink consideration of quantum effects becomes necessary. We consider a single junction between two wires up to a four by four grid of wires. Through a series of calculations with atomistic first-principles, tight-binding and analytic models of multi-terminal devices we demonstrate the presence of unique behavior, such as interference effects, not present in classical models. It is expected that exploitation of these effects will be useful in the creation of circuit components.

Tuesday Morning, November 1, 2011

Electron Transport in Low Dimensional Materials Focus Topic

Room: 209 - Session ET+EM+NS+GR-TuM

Electron Behaviors in Nanoelectronics, Interconnect, and Carbon-based Materials

Moderator: J. Wendelken, Oak Ridge National Laboratory, A. Swan, Boston University

8:00am **ET+EM+NS+GR-TuM1 Electron Transport Study of Graphene on SiC Using Scanning Tunneling Potentiometry.** *K. Clark, S. Qin*, Oak Ridge National Laboratory, *G. He*, Carnegie Mellon University, *G. Gu*, The University of Tennessee, *R.M. Feenstra*, Carnegie Mellon University, *A.-P. Li*, Oak Ridge National Laboratory

The unique electronic and transport properties of graphene have helped this material emerge as a perspective graphene based electronic system. Single layers of graphene formed on SiC look to be a promising system for the realization of graphene electronics. To utilize the full potential of graphene on SiC a complete understanding of the physical and electronic properties of this system is needed. This study uses Scanning Tunneling Microscope (STM) images along with scanning tunneling spectroscopy to characterize the sample surface. STM images clearly show the distinction between 1 monolayer (ML) and 2ML regions. The 1ML to 2ML transition is further confirmed by point spectroscopy measurements and spectroscopic mapping across the boundary. Defects, grain boundaries, step edges and other potential scattering centers are thought to play a major role in the electronic properties, especially in transport, along the graphene sheets. Using a low temperature four-probe scanning tunneling microscope, potentiometry measurements are performed on epitaxial graphene grown on 4H-SiC. Potentiometry maps spanning the transition from 1ML to 2ML graphene layers show a contrast change indicating a potential change at this interface. Preliminary results of the transport along this potentially revolutionary new electronic system will be presented. This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy.

8:20am **ET+EM+NS+GR-TuM2 Engineering the Electronic States of CVD Grown Few Layer Graphene by Twisting and Lattice Distortion.** *M.H. Pan*, Oak Ridge National Laboratory, *X.T. Jia*, *S. Bhaviripudi*, Massachusetts Institute of Technology, *V. Meunier*, Rensselaer Polytechnic Institute, *M.S. Dresselhaus*, *J. Kong*, Massachusetts Institute of Technology
Few layer graphene (FLG) can have advantages over single layer graphene because it has a larger current-carrying capacity and the electronic properties are sensitive to more engineerable system parameters. In particular, Hass et al. have demonstrated that orientational disorder is normally present in carbon-face SiC epitaxial FLG samples. [1] Recently both theoretical and experimental studies suggest that strain can be used to engineer graphene electronic states through the creation of a pseudo-magnetic field. [2] Here we present both scanning tunneling microscopic/spectroscopic (STM/S) studies of chemical vapor deposition grown few layer graphene samples. There indeed exists a twisting between the stacked graphene layers, confirmed by both high-resolution STM images and low temperature spectroscopic measurements. Our results show that, by stretching graphene along three symmetry directions, a strain-induced pseudo magnetic field can lead to the formation of different Charge Density Wave (CDW) states at the top layer of graphene.

[i] Hass, J., Varchon, F., *Phys. Rev. Lett.* **100**, 125504(2008)

[ii] Levy, N. et al., *Science* **329**, 544 (2010).

8:40am **ET+EM+NS+GR-TuM3 Unique One- and Two-Dimensional Phenomena Observed in Carbon Nanotubes and Graphene.** *S. Cronin*, University of Southern California **INVITED**

Our ability to fabricate nearly defect-free, suspended carbon nanotubes (CNTs) has enabled us to observe several phenomena never seen before in CNTs, including breakdown of the Born-Oppenheimer approximation[1], mode selective electron-phonon coupling[2], leading to negative differential resistance (NDR) and non-equilibrium phonon populations, and a Mott insulator transition[3]. In this work, Raman spectroscopy is used to measure individual, suspended CNTs under applied gate and bias potentials. Raman spectroscopy of periodic ripple formation in suspended graphene will also

be reported. As will be shown, preparing clean, defect-free devices is an essential prerequisite for studying the rich low-dimensional physics of CNTs and graphene.

1. Bushmaker, A.W., Deshpande, V.V., Hsieh, S., Bockrath, M.W., and Cronin, S.B., "Direct Observation of Born-Oppenheimer Approximation Breakdown in Carbon Nanotubes." *Nano Letters*, **9**, 607 (2009).
2. Bushmaker, A.W., Deshpande, V.V., Bockrath, M.W., and Cronin, S.B., "Direct Observation of Mode Selective Electron-Phonon Coupling in Suspended Carbon Nanotubes." *Nano Letters*, **7**, 3618 (2007).
3. Bushmaker, A.W., Deshpande, V.V., Hsieh, S., Bockrath, M.W., and Cronin, S.B., "Large Modulations in the Intensity of Raman-Scattered Light from Pristine Carbon Nanotubes." *Physical Review Letters*, **103**, 067401 (2009).

9:20am **ET+EM+NS+GR-TuM5 Probing Surface Band Conduction through Back-Gated Conductance Measurements on Si Nanomembranes.** *W.N. Peng**, *J. Endres*, *S. Scott*, *Z. Aksamija*, *D.E. Savage*, *I. Knezevic*, *M.G. Lagally*, *M. Eriksson*, University of Wisconsin Madison

Silicon-on-insulator substrates provide large-area Si nanomembranes (SiNMs) mechanically supported by bulk handle wafers. Because of the intervening oxides, SiNMs are also electrically isolated from the substrates. The typical membrane thickness is less than a few hundred nanometers. Because they are so thin, SiNMs display interesting transport phenomena influenced by surface effects. Here, we demonstrate a novel method to probe surface transport via conductance measurements on SiNMs. When contacts are placed on the front surface, a current flows between the source and the drain via the membrane body as well as its surface. By utilizing an underlying back gate (the Si handle substrate), the conductance through the membrane can be continuously tuned and made smaller than the surface contribution, enabling experimental determination of the surface conductance. We measure the membrane conductance as a function of both the membrane thickness and the backgate voltage in ultra-high vacuum. In contrast to H-terminated Si surfaces, clean reconstructed Si(001)(2×1) surfaces show a constant-conductance regime when the backgate voltage is varied, and the conductance in this regime does not depend on membranes thickness. We demonstrate that the constant conductance (on the order of 10^{-9} Siemens) stems from an additional conduction channel through the dimer-reconstructed surface π^* band. By comparing the experimental results to numerical simulations, the surface band mobility is determined to be in the range 10-50 cm^2/Vs .

Research supported by NSF [UW MRSEC, award DMR-0520527, as well as awards 0937060 (subaward CIF-146) and ECCS-0547415] and DOE

9:40am **ET+EM+NS+GR-TuM6 Ferroelectric Field-Effect Transistor Behavior in CdS Nanotetrapods.** *S. Qin*, Oak Ridge National Laboratory, *W. Fu*, *L. Liu*, Chinese Academy of Sciences, *T.H. Kim*, Oak Ridge National Laboratory, *S.L. Hellstrom*, Stanford University, *W. Wang*, *W. Liang*, *X. Bai*, *E. Wang*, Chinese Academy of Sciences, *A.-P. Li*, Oak Ridge National Laboratory

Complex nanostructures such as branched semiconductor nanotetrapods are promising building blocks for next-generation nanoelectronics. Here we report on the electrical transport properties of individual CdS tetrapods in a field-effect transistor (FET) configuration with a ferroelectric $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$ film as high- κ , switchable gate dielectric. A cryogenic four-probe scanning tunneling microscopy is used to probe the electrical transport through individual nanotetrapods at different temperatures. A *p*-type field effect is observed at room temperature, owing to the enhanced gate capacitance coupling. And the reversible remnant polarization of the ferroelectric gate dielectric leads to a well-defined nonvolatile memory effect. The field effect is shown to originate from the channel tuning in the arm/core/arm junctions of nanotetrapods. At low temperature (8.5 K), the nanotetrapod devices exhibit a ferroelectric-modulated single-electron transistor behavior. The results illustrate how the characteristics of a ferroelectric such as switchable polarization and high dielectric constant can be exploited to control the functionality of individual 3-dimensional nano-architectures. *Acknowledgement:* The research at the Center for Nanophase Materials Sciences is sponsored at Oak Ridge National Laboratory by the Office of Basic Energy Sciences, U.S. Department of Energy. The research in Beijing is supported by MOST and CAS of China.

* NSTD Student Award Finalist

10:40am **ET+EM+NS+GR-TuM9 Probing Electron-Electron Correlations in Quantum Dots Using Transport: Quantum Monte Carlo Studies, H.U. Baranger, Duke University** **INVITED**

Strong electron-electron correlations occur in nanoscale systems in a variety of contexts – when electrons form a crystal at low density, for example, or in correlations between quantum dots. Nanoscale systems introduce in addition an unprecedented level of control over the physical parameters determining such correlations. As electron transport is one of the primary probes of nanosystems, the effect of e-e correlations on transport is a key issue. I shall discuss an example in which we used quantum Monte Carlo (QMC) techniques to calculate the conductance:

Consider a system of four quantum dots designed to study the competition between three types of interactions: Heisenberg, Kondo, and Ising. We find that the competition produces a rich phase diagram containing two sharp features: a quantum phase transition (QPT) between charge-ordered and charge-liquid phases, and a dramatic resonance in the charge liquid visible in the conductance. The conductance is calculated using a world-line QMC method: extrapolation of the imaginary time QMC data to zero frequency yields the linear conductance, which is then compared to numerical renormalization group results in order to assess its accuracy. The QPT is of the Kosterlitz-Thouless type with a discontinuous jump in the conductance at the transition. We connect the sharp resonance phenomenon with the degeneracy of three levels in the isolated quadruple dot and argue that this leads to an emergent symmetry. I shall end by discussing the sensitivity to parameter variation and possible experimental realizations in laterally gated quantum dots as well as carbon nanotubes.

This work was done in collaboration with Dong E. Liu and Shailesh Chandrasekharan (Duke University).

11:20am **ET+EM+NS+GR-TuM11 Resistivity Increase due to Electron Scattering at Surfaces and Grain Boundaries in Metal Thin Films and Nanowires, J.S. Chawla, D. Gall, Rensselaer Polytechnic Institute**

The effect of surface and grain boundary scattering on the resistivity of Cu thin films and nanowires is quantified using (i) *in situ* transport measurements on single-crystal, atomically smooth Cu(001) layers, (ii) textured Cu(111) layers and patterned Cu wires with independently varying grain size, thickness and line width, and (iii) *in situ* grown interfaces including Cu-Ta, Cu-MgO, Cu-SiO₂ and Cu-oxygen. In addition, the electron surface scattering is also measured *in situ* for single-crystal Ag(001) and TiN(001) layers. These findings are important for the development of future generation narrow low-resistivity Cu interconnects and TiN metal gates.

Cu(001), Ag(001), and TiN(001) layers with a minimum continuous thickness of 4, 5 and 1.8 nm, respectively, are grown by ultra-high vacuum magnetron sputter deposition on MgO(001) substrates and are found to be atomically smooth single crystals by a combination of x-ray diffraction θ - 2θ scans, ω -rocking curves, pole figures, reciprocal space mapping, Rutherford backscattering, x-ray reflectometry, transmission electron microscopy, and *in-situ* scanning tunneling microscopy. Polycrystalline Cu layers with a 111-texture are deposited on thermally grown SiO₂, with and without Ta barrier layer. Subsequent *in-situ* annealing at 350°C followed by sputter etching in Ar plasma yields Cu layers with independently variable thickness and grain size. Cu nanowires, 50 to 150 nm long, 70 to 350 nm wide, and 45 nm thick, are patterned using electron beam lithography and sputter etching.

In-situ electron transport measurements at room temperature in vacuum and at 77 K in liquid nitrogen for single-crystal Cu and Ag layers is consistent with the Fuchs-Sondheimer (FS) model and indicates specular scattering at the metal-vacuum boundary with an average specularly parameter $p = 0.6$ and 0.4, respectively. In contrast, layers measured *ex-situ* show completely diffuse surface scattering due to sub-monolayer oxidation. Electron transport measurements for polycrystalline Cu/Ta layers and wires show a ~10% and ~11% decrease in resistivity, respectively, when increasing the average lateral grain size by factor 2. *In-situ* deposition of 0.3 to 8 nm thick Ta barrier layers on Cu(001) leads to a resistance increase that indicates a transition from $p = 0.8$ to $p = 0$, independent of the Ta thickness. *In-situ* exposure of Cu(001) layers to O₂ between 10⁻³ and 10⁵ Pa-s results in a sequential increase, decrease and increase of electrical resistance which is attributed to specular surface scattering for clean Cu(001) and for surfaces with a complete adsorbed monolayer, but diffuse scattering at partial coverage and after chemical oxidation.

11:40am **ET+EM+NS+GR-TuM12 Control of Contact Formation via Electrodeposition on GaAs Nanowires, C. Liu, O. Einabad, S. Watkins, K.L. Kavanagh, Simon Fraser University, Canada**

Copper (Cu) electrical contacts to as-grown gallium arsenide (GaAs) nanowires have been fabricated via electrodeposition. The nanowires are zincblende (111) oriented grown epitaxially on n-type Si-doped GaAs(111)B

substrates by gold-catalyzed Vapor Liquid Solid (VLS) growth in a metal organic vapour phase epitaxy (MOVPE) reactor. The epitaxial electrodeposition process, based on previous work with bulk GaAs substrates, consists of a substrate oxide pre-etch in dilute ammonium hydroxide carried out prior to galvanostatic electrodeposition in a pure Cu or Fe sulphate aqueous electrolyte at 20°C. The conductivity of wires was controlled via the addition of carbon tetrabromide (CBr₄) during growth. For nominally undoped GaAs nanowires, we find that Cu or Fe has a preference for growth on the gold catalyst avoiding the sidewalls. After etching the gold, both metals still preferred to grow only on the tops of the nanowire, consistent with the location of the largest electric field. Core-shell GaAs nanowires with highly conductive carbon-doped shells were fabricated via changing the Ga precursors from triethylgallium to trimethylgallium for radial growth. Increasing the conductivity of the nanowires in this way, not surprisingly; meant that Cu nucleation and growth began to occur on the sidewalls as well as on the gold catalyst. Finite element simulations will be compared to our electrodeposition results towards the calibration of nanowire conductivity.

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