The Effect of Annealing on the Spin-Transfer Torques of Magnesium Oxide Magnetic Tunneling Junction Nanopillars

CNF Project # 111-80
Principal Investigator(s): Robert A. Buhrman
User(s): Yun Li

Affiliation(s): School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853
Primary Research Funding: NSF
Contact: rab8@cornell.edu, YL425@cornell.edu

Abstract:

Thermal annealing is essential for enhancing the tunneling magnetoresistance (TMR) of magnetic tunnel junctions (MTJs), and many studies have focused on the effect of annealing on MTJ chemical, structural, and electrical transport properties [1-3]. Here, we report the magnetic, electronic properties and the in-plane and field-like spin-transfer torques (STT) in both as-grown and post-annealed FeCoB/MgO/FeCoB MTJs nanopillars. We find that the 350°C vacuum annealing breaks the symmetry of the bias dependence of the TMR, conductivity, and switching phase diagram (SPD). This STT change is consistent with the change in chemical composition and structural coherency of the MTJ interfaces and electrodes, indicated by XRD and analytical STEM analyzes.

Summary:

In this report, we study magnesium oxide (MgO)-based MTJs of the composition (thickness in nanometers) bottom contact / IrMn (10) / CoFeB (2) / MgO (1) / CoFeB (1.5) / top contact. We grew the thin film stacks on 3-inch thermally oxidized Si wafers in a vacuum system containing multiple magnetron sputtering sources. The top CoFeB was patterned by e-beam lithography and ion beam etching technique to produce an elliptical cross-section with a nominal size of 200 × 120 nm² for spin transfer switching measurement (Figure 1). The resistance-area product for the parallel configuration in our as-grown MTJs (annealed) is about 16Ω*µm² (20Ω*µm²). The etching was stopped at the MgO barrier and thus the bottom layer is largely unpatterned to minimize the stray field from the bottom ferromagnetic electrode. After the patterning process, some of the MTJs were measured directly and some were annealed at 350°C for one hour under an easy-axis magnetic field of 2T in vacuum to enhance the TMR. Each measurement was carried out on three samples and show similar results, while the data presented in this letter are from just one sample.

Figure 1: AFM image of nanopillar array.
Figure 2 shows the switching behavior. The annealing process enhances TMR from about 13% to 90%, indicating a 120% increase in the tunnel current polarization from ~25% to ~56%. The annealed (as-grown) sample can achieve bipolar current driven switching with bias pulses of 20 ms in for an applied magnetic field of 35 Oe (54 Oe).

To investigate the switching properties of the devices and to evaluate the STT amplitude, we first measured the switching phase diagram (SPD), where the coercive field ($H_c$) is measured as the function of DC bias (Figure 3). The boundary of the SPD is rather symmetric about the zero point of the coordinate for the as-grown sample, while this symmetry is markedly broken after annealing. The PSD provides an intuitionistic picture of the spin transfer torque: qualitatively the locations of the points of intersection of the curves are determined by the STT. Specifically, the voltage intersection point is determined by the magnitude of the in-plane torque (IPT) and the magnetic field location of the intersection point is determined by the magnitude of the field-like torque (FLT). A larger IPT will cause the boundary curves to cross at a lower voltage and a stronger FLT will make the curves bend towards the negative field direction since the FLT, or the interlayer exchange coupling, generally acts to promote the antiparallel alignment of the magnetic moments of the ferromagnetic electrodes of the MTJs. Therefore we conclude that annealing enhances the asymmetry of the bias dependent IPT and increases the magnitude of the FLT as indicated by our SPD plots.

References:

Abstract:
We designed and fabricated a three-terminal spin transfer torque device in which combines a Co$_{40}$Fe$_{40}$B$_{20}$/Cu/Co$_{40}$Fe$_{40}$B$_{20}$ spin valve and a Co$_{40}$Fe$_{40}$B$_{20}$/MgO/Co$_{40}$Fe$_{40}$B$_{20}$ magnetic tunnel junction (MTJ) with a common Co$_{40}$Fe$_{40}$B$_{20}$ free layer. Conventional two-terminal devices were also studied in order to optimize the performance of our final device. Switching current density $J_s \approx 3 \times 10^7$ A/cm$^2$ in spin valve and tunneling magnetoresistance (TMR) $\approx 140\%$ in MTJ were observed in these stand alone samples.

Summary:
Magnetic tunnel junctions (MTJ) and spin valves are two promising candidates for future magnetic random access memory (MRAM) devices that have been widely studied for the past few years [1,2]. By utilizing spin transfer torque (STT) effect, pure electrical switching of the magnetic configurations of nano-scale MTJs and spin valves can be realized with critical current density $\approx 10^6 - 10^7$ A/cm$^2$ [3-5]. Although STT-MTJ MRAM has the advantage of higher magneto-resistance (MR) ratio while comparing to its spin valve counterpart, dielectric breakdown of ultrathin (1-2 nm) tunnel barrier and unreliable switching caused by back-hopping of MTJs at higher applied voltages ($\approx 1$V) are undesirable for industrial applications [5, 6]. In order to bypass these issues, several three-terminal devices have been proposed and studied [7,8]. Here we demonstrate the fabrication of a three-terminal spin transfer torque device which is similar to the structure in our previous work [7] but with a different nano-fabrication process and a much simpler spin valve layer design. A schematic topology of our device is shown in Figure 1. The left and the right top leads are the writing ports while the right top lead and bottom lead comprise the reading ports. The free switching ferromagnetic layer (double headed arrow in Figure 1) is shared by the spin valve and the MTJ. Both fixed ferromagnetic layers (single headed arrows) are pinned by antiferromagnetic Ir$_{20}$Mn$_{80}$ (IrMn) layers. Cu spacer and MgO tunnel barrier are used in spin valve and MTJ, respectively. All three ferromagnetic layers are Co$_{40}$Fe$_{40}$B$_{20}$ (CoFeB).

Figure 1: A schematic illustration of three-terminal STT device. Writing current is sent through top electrodes to introduce a spin transfer torque on common free layer (double-headed arrow). Reading is done by measuring the TMR between top and bottom electrodes.

Figure 2: SEM of a typical device before patterning top electrodes.
The layer stacks (in nm) bottom layers / IrMn(20) / CoFeB(5) / MgO(wedge) / CoFeB(4) / Cu(8) / CoFeB(5) / IrMn(20) / capping layers were first deposited by sputtering under 2 mTorr. The film was then fabricated into designed structure by multiple steps of aligned e-beam lithography and ion-milling. An elliptical shape pattern with dimensions ~ 80 nm x 200 nm was first defined by e-beam lithography and then milled down to the bottom IrMn layer. Second e-beam lithography was used to pattern a milling mask with its edge at the middle of the device. The right half of the device was then ion-milled to the CoFeB free layer. In order to connect top electrodes precisely out from the two ends of the device, a third aligned e-beam exposure is required. Scanning electron microscope (SEM) image of a typical device before patterning top electrodes is shown in Figure 2. Bottom lead was defined separately by photolithography afterwards. E-beam evaporated silicon oxide was used as insulating and protection layer of the device.

In order to characterize the behavior and to optimize the performance of our final design, stand-alone CoFeB/Cu/CoFeB spin valves and CoFeB/MgO/CoFeB MTJs were also fabricated and examined. Figure 3 (a) and (b) are the resistance-to-current data from DC 2-probe measurements which indicate the switching properties of a typical CoFeB/Cu/CoFeB spin valve with similar dimensions (70 nm x 200 nm) to our three-terminal device. The critical currents for switching from anti-parallel (AP) state to parallel (P) state and from P to AP are \( J_{cAP} \rightarrow P \sim 2.3 \times 10^7 \text{A/cm}^2 \) and \( J_{P} \rightarrow AP \sim 3.8 \times 10^7 \text{A/cm}^2 \), respectively. On the other hand, as growth MTJ samples show TMR ~ 30% and reaches ~ 140% after magnetic annealing at 350°C for 30 minutes. HR loop measurement of a typical 70 nm x 200 nm MTJ sample after annealing is shown in Figure 4.

References:
High Voltage Pulse Measurement of Microwave Emission and Spin-Torque Effects in Magnetic Tunnel Junctions

CNF Project # 111-80
Principal Investigator(s): Robert A. Buhrman
User(s): Hsin-wei Tseng, Yun Li, Praveen Gowtham

Affiliation(s): School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14850
Primary Research Funding: ONR, CCMR, CNS, NSF
Contact: rab8@cornell.edu, ht229@cornell.edu

Abstract:

Ultrafast spin-transfer switching in MgO-based magnetic tunnel junctions (MTJs) requires high pulse voltage (~ 1V). High voltage switching, however, easily resulted in unreliable switching. The physics behind unreliable switching is still not very well understood in MTJs. Here, we report pulse-based microwave measurement which enables us to directly probe the microwave dynamics and switching behaviors of MgO MTJs. We associated unreliable switching with incoherent microwave oscillation in free layers. Highly asymmetric microwave emission and unreliable switching can be explained by fieldlike torque. Even fieldlike torque is not as strong as in-plane spin torque, its effect completely changes the magnetic dynamics at high voltage at zero effective field and induces the unreliable switching events under high voltage bias.

Summary of Research:

Spin-transfer torque (STT) enables electric manipulation of nanomagnets and has been extensively studied due to its application in ultrafast non-volatile storage technology, especially STT-based magnetic random access memory (STT-MRAM). STT-MRAM is one candidate for future non-volatile memory technology, due to its ultrafast switching speed (~ 1 GHz) and scalability. Achieving ultrafast switching requires shorter pulses. Therefore, higher pulse voltages are needed.

At high voltages, however, unreliable switching behavior under specific current polarities have been reported, including backhopping and abnormal switching. Those issues hindered the commercialization of STT-MRAM. Resolving those issues requires understanding of spin-transfer physics at high voltage bias. Many researches have used various techniques to reveal the spin-transfer torque. Spin-transfer torque is still not very well understood under high voltage (~ 1V) for ultrafast switching.

Here, we utilize the strong microwave emission of MgO-based MTJs. We are able to directly probe the nanomagnet dynamics of CoFe-based MgO nanopillar MTJs under high voltage (~ 1V) through pulse-based technique. With this pulse-based microwave measurement, we have obtained information which has not been reported before. Highly asymmetric spin-transfer torque excited dynamics under different current directions and strong voltage dependence of dynamics behaviors are observed (see Figure 1). We have furthermore established the relationship with microwave power phase diagram and switching diagram (See Figure 2).

Pulse-based microwave measurement has revealed highly asymmetric spin-transfer effects under high voltage polarities (1V) in MgO-based MTJs for first time. Free layer goes to chaotic motion at high bias, suggesting strong in-plane and opposite fieldlike torque V < 0 would lower the thermal barrier (due to reduction of Hk) and result in backhopping. As V > 0, fieldlike torque quench the oscillation and confine the nanomagnet (enhance magnetic anisotropy), resulting in coherent oscillation and reliable switching.

Our results have important implication that while pushing for ultrafast switching, higher voltage is required. Fieldlike torque could affect high voltage spin-transfer effect resulting unreliable switching for AP-to-P switching and enhance the switching for P-to-AP. Simply reducing saturation magnetization will easily resulted in chaotic motion under high voltage; therefore, resulted in unreliable switching. For the future design, it might require large coercivity to suppress fieldlike torque effect under high voltage or controlling the effects of fieldlike torque in MTJs.
References:

Fabrication of Charge-Density-Wave Conductor Field Effect Devices

CNF Project # 316-87  
Principal Investigator(s): Robert Thorne  
User(s): Ethan Geil  
Affiliation(s): Laboratory of Atomic and Solid State Physics, Cornell University  
Primary Research Funding: NSF DMR 0805240  
Contact: ret6@cornell.edu, ecg33@cornell.edu

Abstract:

We are fabricating MOSFET-like devices using the charge-density-wave (CDW) conductor niobium triselenide (NbSe₃) as the channel. The gate voltage produces a small modulation of the single-particle resistivity and a much larger modulation of the threshold field for CDW motion and thus of the conductance of the collective mode.

Summary of Research:

Niobium triselenide undergoes two Peierls transitions at 145 K and 59 K. Each transition opens a gap along part of the Fermi surface, and a fraction of the carriers condense into a charge-density wave [1,2]. The CDW is pinned by impurities, so it does not participate in conduction at low fields. At a threshold field $E_T$, however, the density wave depins and contributes to the total conduction. This gives rise to the I-V characteristic shown in Figure 1.

To investigate the effect of a transverse electric field on CDW conduction, we have fabricated MOSFET-like devices [3], diagrammed in Figure 2. A 70 nm layer of dry thermal oxide was grown on a degenerately doped (P++) silicon substrate. Gold contact pads were patterned using an evaporation/liftoff technique. For each substrate, a thin, freshly cleaved ribbon (~ 0.1 - 1 µm thick) of NbSe₃ was carefully laid down on the oxide and connected to the gold pads using either indium wires or silver conductive paste. This structure effectively forms a capacitor, with the NbSe₃ as one plate and the bulk silicon as the other. Due to the high carrier density (3.8 x 10²¹ cm⁻³) of this material, it is necessary to use very thin samples in order to get a reasonable charge modulation. A gate voltage ($V_{gs}$) was applied between the substrate silicon and the source pad, and a bias ($V_{ds}$) was applied between the source and drain pads. Curves of the source-drain current $I_{ds}$ vs. $V_{gs}$ were measured at various values of $V_{gs}$. The room-temperature resistivity of a typical sample ($\rho_{rs} / I_{ds}$) varies with gate voltage. The sign and magnitude are consistent with hole-type conduction.

Figure 3 shows I-V curves for several gate voltages at $T = 30$ K, below both transitions. Despite the relatively small change in carrier density, there is a large modulation of the threshold field for CDW conduction and thus of the collective conductance. The mechanism responsible for this large modulation is uncertain, but may be related to pinning of field-induced edge dislocations. These devices are being used to investigate CDW-single particle interactions and pinning-based data storage.

References:


Figure 1: I-V characteristic of a CDW conductor. Below $E_{r}$, the CDW is pinned by impurities. Above $E_{r}$, the CDW slides and contributes to the total current. The single particle current is due to ohmic conduction of electrons along the ungapped portion of the Fermi surface and of single-particle excitations in the gapped portion.

Figure 2: Field-effect device. A voltage is applied between the substrate and the single crystal NbSe₃ channel, and I-V curves for the channel are measured.

Figure 3: I-V data versus gate voltage at $T = 30$ K, for the $T_{c} = 59$K CDW. Although the modulation of the carrier density and single-particle conductance is small, the modulation of threshold for CDW conduction and collective motion is large.
Giant Proximity Effects in Confined Superfluid 4He

CNF Project # 526-94
Principal Investigator(s): Francis M. Gasparini
User(s): Justin K. Perron

Affiliation(s): Department of Physics, University at Buffalo
Primary Research Funding: National Science Foundation
Contact: fmg@buffalo.edu, jkperron@buffalo.edu
Web Site: http://enthalpy.physics.buffalo.edu

Abstract:

Previous measurements of the specific heat of 4He confined in all three spatial dimensions suggested a coupling between neighboring confinements through the tiny channels used to fill them [1]. Measurements of the superfluid fraction in the filling channels also suggested an enhancement attributed to their proximity to the larger regions of superfluid [1]. Recent measurements of confinement structures designed at the Cornell NanoScale Facility (CNF) have confirmed these effects [2], and begun to address their nature [3].

Summary of Research:

Using the facilities at CNF, we are able to etch various geometries out of thermally grown silicon oxide. Then, through direct wafer bonding of two patterned wafers, we have been able to construct extremely uniform and well-characterized confinement cells (see Figures 1 and 2). Measurements of the specific heat and superfluid fraction of liquid helium in these confinements has allowed, for the first time, observation of coupling between neighboring confinements as well as proximity effects on a thin film in equilibrium with larger regions of superfluid [2].

Specific heat data for an array of (1 µm)³ confinements showed various anomalies [4]. It was suggested that these anomalies could be explained by a coupling between the confinements through the small channels used to fill them [1]. This coupling reveals itself as an enhancement in the specific heat. A measurement of (2 µm)³ confinements has allowed us, via scaling, to quantify this enhancement (Figure 3) [2].

The (2 µm)³ measurement also identified proximity effects on the 31.7 nm film used to fill the (2 µm)³ boxes [2]. These proximity effects include an increase in both the superfluid fraction and the specific heat of the film, as well as an increase in the temperature of the specific heat maximum, and the

Figure 1: Confinement Cell. A diagram (not to scale) of a cell used to confine liquid helium. This consists of an array of (2 µm)³ boxes etched in a thermally grown oxide on a 2-inch silicon wafer. A second wafer has an outer wall and several support posts etched into a 31.7 nm oxide. This wafer forms a uniform film used to fill the (2 µm)³. After patterning of the silicon wafers they are bonded together and form a confinement cell to be filled with helium.

Figure 2: Confinements. An scanning electron microscope image of (2 µm)³ boxes etched out of thermally grown silicon oxide. These boxes are filled with liquid helium creating an extremely well defined array of uniform confinements.
temperature of the superfluid onset (Figure 4) [2]. These proximity effects are analogous to similar effects seen in superconducting sandwiches with one apparent difference. The standard model for proximity effects in superconductors allows for the effects to occur over distances comparable to the correlation-length $\xi$ of the system, however in our case we observe these effects across distances over 100 times $\xi$. This has mirrored recent measurements of a “giant proximity effect” in high temperature superconductors [5]. Although these measurements cannot be explained using the standard theory for superconducting proximity effects, recently a group has proposed an explanation involving phase fluctuations [6]. It is believed that the analogous effect measured by our group may owe itself to a similar mechanism.

Our current work involves changing the periodicity of the (2 $\mu$m)$^3$ boxes in equilibrium with the 31.7 nm film in order to correlate the periodicity with the magnitude of the proximity effects. This will shed some light on the nature of these effects, as well as determine if the mechanism from Ref. [5] can be applied to the liquid helium system.

References:


Figure 3: Cp Coupling. A plot of an enhancement in specific heat of (1 $\mu$m)$^3$ boxes due to coupling between neighboring confinements. This is calculated via scaling using data from uncoupled (2 $\mu$m)$^3$ boxes.

Figure 4: Superfluid Fraction. Plot of the superfluid fraction $\rho_s/\rho$ vs. reduced temperature $t = (T - T_\lambda)/T_\lambda$ for two different confinements. A uniform 48.3 nm film and a uniform 31.7 nm film in equilibrium with (2 $\mu$m)$^3$ boxes. Also shown are the values for $t_c$ predicted from two dimensional scaling data[3]. The data for the 31.7 nm confinement shows $\rho_s/\rho$ persisting to a higher temperature than expected. The nature of this effect is one of the primary goals of our group’s current research.
X-Ray Imaging of Magnetic Normal Modes Driven by Spin Transfer Torque in Magnetic Nanopillar Devices

CNF Project # 598-96
Principal Investigator(s): Daniel C. Ralph\textsuperscript{2}, Robert A. Buhrman\textsuperscript{1}
User(s): Yongtao Cui\textsuperscript{1}, Lin Xue\textsuperscript{2}

Affiliation(s): 1. Applied and Engineering Physics, 2. Department of Physics; Cornell University
Primary Research Funding: Army Research Office; MURI, National Science Foundation; Division of Materials Research, and National Science Foundation; Nanoscale Science and Engineering Centers
Contact: ralph@ccmr.cornell.edu, rab8@cornell.edu, yc368@cornell.edu, lx39@cornell.edu

Abstract:

We have fabricated CoFe/Cu/NiFe magnetic nanopillars with $100 \times 250$ nm$^2$ elliptical cross section on top of a suspended silicon nitride membrane, designed for performing x-ray transmission microscopy of magnetic dynamics. We are now studying these devices to image the magnetic normal modes that can be excited by the spin transfer torque from a microwave-frequency current passing through the pillar.

Summary of Research:

A spin-polarized current passing through a ferromagnet can exert a torque on the ferromagnet that is strong enough to either reverse its magnetization or excite steady-state high-frequency (1-20 GHz) magnetization precession, depending on the device structure and applied magnetic field [1]. This spin-torque effect is under intensive study both because of its fundamental importance and because of its potential applications in magnetic random access memory (MRAM) and high speed signal processing. One of the critical outstanding issues in this field is the nature of the magnetization dynamics excited by the spin torque. Direct imaging [2,3] of the spatial and temporal dependence of the magnetic dynamic modes with high resolution x-ray transmission microscopy can offer unique understanding of this effect and would be a major advance in this field. X-ray transmission microscopy can selectively image a ferromagnetic element via x-ray magnetic circular dichroism (XMCD), by which the transmission of x-ray photons through a ferromagnetic material depends on the polarization of the photons and the magnetization direction of the ferromagnetic element.

Figure 1: Device schematic: nanopillar device on top of a suspended silicon nitride membrane.

Figure 2: Spin-transfer-driven ferromagnetic resonance spectra of one device.
We start with a Si substrate coated with 150 nm low stress (film tension < 200 MPa) SiN films on both sides, one of which will be made into suspended membrane to allow for x-ray transmission microscopy (Figure 1).

We deposit the metallic multilayers of the structure (in nm): \{Ta 3 / CuN 20\}_2 / Ta 3 / Py 40 / Cu 6 / Co_{80}Fe_{10} 15 / Cu 4 / Ru 4 (where Py is the magnetic alloy permalloy, Ni_{81}Fe_{19}) in a sputtering system. E-beam lithography and ion milling are then used to define pillars with elliptical cross section of 100 × 250 nm² (Figure 2). Multiple steps of photolithography and ion milling are used to make the contact leads, and silicon oxide is deposited by electron-beam evaporation to provide electrical isolation between top and bottom leads. To form the suspended nitride membrane, the Si substrate is etched anisotropically in heated KOH solution, using photolithographically-patterned silicon nitride on the back side of the substrate as the etch mask.

The XMCD experiments are carried out at the full-field soft x-ray transmission microscope (XM-1) and the scanning transmission x-ray microscope (STXM) at the Advanced Light Source of Lawrence Berkeley National Laboratory. Both microscopes have a spatial resolution of 15 nm and temporal resolution of 70 ps. The x-ray is incident at 30° from the normal direction of the device plane (Figure 1), and its energy is tuned to the characteristic Co L₃ resonance absorption edge. These experiment conditions allow detection of the in-plane component of the magnetization at 15 nm thin CoFe layer in the nanopillar cross-section. A magnetic field is applied in the device plane along the short axis of the ellipse.

Figure 2 shows the electrical characterization of the spin-transfer-driven ferromagnetic resonance [4] spectrum of one sample as a function of microwave current frequency, f, and magnetic field, H. For x-ray studies, we excite the sample into a particular resonance mode with appropriate values of f and H (for example, point A around 2.5 GHz in Figure 2), and use x-ray microscope to image the spatial configuration of the magnetization at 8 different phases (phase 1 to 8) evenly spaced throughout one oscillation cycle. Magnetic contrast images are shown in Figure 3. Figure 3a (b, c, d) corresponds to the contrast between phase 1 (2, 3, 4) and phase 5 (6, 7, 8).

The contrast images show that the magnetic precession is not uniform within the nanopillar -- the lower edge precesses at a different phase and amplitude than the center of the device. We are currently working on imaging the resonance modes at higher frequencies and comparing with micromagnetic simulations to understand the mode structure in these 15 nm CoFe devices. We are also planning to investigate samples with thinner (5 nm) magnetic layer in which the results can be directly compared to previous electrical studies of spin-transfer-driven magnetic dynamics.

References:

Nanoscale Superconducting Microwave Cavities for Ferromagnetic Resonance Studies

CNF Project # 598-96
Principal Investigator(s): Daniel C. Ralph
User(s): Ted Gudmundsen

Affiliation(s): Physics Department, Cornell University
Primary Research Funding: NSF/GRFP, NSF/DMR, NSF/NSEC
Contact: ralph@ccmr.cornell.edu, ted.gudmundsen@gmail.com
Web Site: http://people.ccmr.cornell.edu/~ralph

Abstract:

We have fabricated superconducting microwave cavities with 250 nm nanometer gap sizes to allow ferromagnetic resonance studies of nanomagnets with increased sensitivity.

Summary of Research:

Nanomagnets, ferromagnetic metals that have been manufactured to nanoscale dimensions, have widespread application in digital memory, for example in the read head sensors within hard disk drives. Understanding the properties and dynamics of nanomagnets is important for future progress in information storage. One way to study these properties and dynamics is by applying oscillating magnetic fields at the nanomagnet’s resonant frequency and observing the nanomagnet’s response. This frequency is in the gigahertz, or microwave range. Microwave cavities are useful for amplifying such oscillating magnetic fields, for that reason, ferromagnetic resonance (FMR) experiments have used microwave cavities for 50 years [1].

More recently, superconducting microwave cavities based on thin-film coplanar waveguide have been introduced for measuring the position of nanomechanical resonators [2,3] and for coupling qubits based on Josephson junctions [4,5,6], but this new technology has not been applied for FMR studies. These cavities have a very large $Q$ ($= 10^6$), which makes it possible to use them for extremely sensitive measurements. The aim of this project is to fabricate superconducting microwave cavities optimized to examine the properties of nanomagnets that are too small for conventional FMR techniques.
Figure 2 shows a close up of a high-$Q$ cavity that we have fabricated out of niobium. The cavity is a thin-film coplanar waveguide made of niobium on a resistive silicon substrate with breaks at each end that serve as mirrors for microwaves. The center niobium line is 480 nm wide, and the gaps on either side are 250 nm wide. The cavity is fabricated as follows.

First, the niobium is sputtered onto the silicon substrate. Photoresist is appropriately patterned with the ASML DUV Stepper, then the niobium is etched using a reactive ion etch. The image was taken on the Zeiss Supra SEM. Before making electrical measurements, the cavities need to have gold pads added to the electrodes on each end in order to facilitate wire bonding—these gold pads are defined photolithographically. In future work, we will characterize the electrical properties of the superconducting cavities and integrate them with nanomagnet devices like those that have been previously fabricated by our research group [7].

References:

Fabrication of Mechanically-Adjustable Devices with Two Opposing Graphene Electrodes

CNF Project # 598-96
Principal Investigator(s): Daniel C. Ralph
User(s): Wan Li

Affiliation(s): Physics Department, Cornell University
Primary Research Funding: NSF/CCI, NSF/DMR
Contact: ralph@ccmr.cornell.edu, WL285@cornell.edu

Abstract:

The goal of this project is to fabricate mechanically-adjustable devices with two face-to-face graphene electrodes. The design of the devices will allow us to perform electrical measurements of molecules spanning between the graphene electrodes while varying the distance between the graphene electrodes and also simultaneously carrying out optical microscopy/spectroscopy through the graphene. Microfluidic channels are designed to bring in liquid solutions of interest to the space between the opposing graphene sheets. This report presents the structure of the device, the fabrication scheme, and our recent progress.

Summary of Research:

Figure 1 shows the schematic of our device. The central part of this device consists of two opposing suspended graphene sheets initially separated by a distance of hundreds of nanometers. The graphene sheets are contacted by metal wires for electrical measurements, and suspended over small holes to allow for simultaneous optical microscopy and spectroscopy. We also incorporate microfluidic channels connected with inlet and outlet ports, which will enable us to bring in liquids of interest to the space between the opposing graphene sheets. A previous study (Ref. 1) demonstrated that with the application of external pressure, suspended graphene sheets can be deflected by over 150 nm. Our device will combine this ability with the opposing graphene geometry, deflecting the graphene sheets together with external pressure to vary the distance between them in a controlled manner. Novel types of experiments will be enabled by this design while taking advantages of the unique high conductivity, transparency, and mechanical strength of graphene.

Figure 2 illustrates the process flow that we are developing to realize the device. The devices are fabricated with two wafers that respectively support the top and bottom graphene sheets. These two wafers are prepared separately, and then bonded together to achieve the final opposing graphene geometry. To prepare the wafer supporting the bottom graphene, we start with a 4 inch silicon wafer coated with 300 nm low stress silicon nitride on both sides. We first pattern the silicon nitride on one side of the wafer and use it as a mask for KOH etching to suspend a SiN membrane on the other side of the wafer create 100 × 100 μm²
Figure 2: Fabrication process flow.

Figure 3: Current Progress: a. Scanning electron micrograph of a suspended graphene sheet on device, inset: diffraction pattern taken on a piece of graphene prepared in the same method as the one on device; b. Current-voltage curve measured between two metal leads contacting with the same piece of graphene; c. Optical micrograph of the a microfluidic channel made by bonding two blank wafers with patterned SU-8; d. Optical image of a test device which was made by bonding a completed bottom wafer to a transparent blank wafer.

windows (Figure 2a). Following this, we define multiple metal leads on the wafer using photolithography (Figure 2b). Small holes to be used for suspending the graphene are then etched on the suspended silicon nitride membrane using CHF$_3$/O$_2$ plasma (Figure 2c), producing hole diameters ranging from 4 to 6 µm. At this stage, the wafer is ready for graphene transfer. To increase the yield of suspended graphene and maintain a relatively clean graphene surface, CVD graphene grown on copper foil is transferred onto the wafer using the method used in Ref. 2, which removes the PMMA on graphene by thermal annealing instead of organic solvents (Figure 2d). The wafer supporting the top graphene is prepared following similar procedures, except that additional windows are opened in the wafer during the KOH etching step to expose the metal leads on the bottom wafer after bonding, and also to permit the introduction of microfluidic inlets/outlets (Figure 2f). No metal leads are defined on the top wafer before bonding.

After the two wafers are prepared, SU-8 is spin-coated on the bottom wafer. Microfluidic channels are patterned into the SU-8 layer using photolithography (Figure 2e), and the two wafers are bonded together using SU-8 as the adhesive layer (Figure 2i). As the last step of fabrication, the top graphene sheet is connected with metal leads by e-beam evaporation using shadow masks (Figure 2j).

Figure 3 shows our current progress on fabrication. Up to now, we have succeeded in obtaining relatively clean graphene sheets suspended over holes on silicon nitride membranes (Figure 3a) with high yield. The contact resistance between the metal leads and graphene is measured to be ~ 250 Ohms (Figure 3b). We also developed a bonding recipe which can bond two blank wafers using SU-8 patterned with microfluidic channels (Figure 3c). We are now working on applying this recipe to bond the wafers that support the top and bottom graphene sheets. Figure 3d shows the optical image of a test device which is made by bonding a completed bottom wafer with a transparent, blank wafer.

References:

Abstract:
We report the experimental observation of spin transfer torque oscillations in a hybrid structure consisting of two in-plane oriented free layers sandwiched with two perpendicularly oriented polarizers with each ferromagnetic layer separated by a non-magnetic spacer. Due to a strong coupling between the in-plane oriented free layers and the spin torque from the perpendicular polarizers, without any external applied magnetic field, we observe high frequency (larger than 6.5 GHz) microwave signals with a minimum linewidth of 74 MHz. The micromagnetic simulations show that the origin of the excitation is characterized by a spatially inhomogeneous dynamics synchronized via magnetostatic coupling and spin-transfer torque. The oscillation mechanisms observed in this device geometry are promising for future development of spintronic microwave oscillators comprising altogether many features such as operation at zero external magnetic field, frequency doubling, and a reduced linewidth due to phase locking between the two magnetic free layers.

Summary of Research:
Spin-torque oscillators (STOs) are nano-scale magnetic devices that are interesting because they can act as frequency-tunable microwave sources and because they can serve as a model system for studying fundamental issues associated with the strongly nonlinear dynamics in nanomagnets [1,2,3]. To see if the properties of STOs can be made superior to other microwave oscillator technologies, it is necessary to optimize the STO performance, with some of the important metrics being broad-band frequency tunability, a narrow spectral linewidth, microwave emission for zero applied magnetic field, and large output power. In this project, we investigate a new STO design which consists of two in-plane oriented free layers sandwiched in between two perpendicularly oriented polarizers, with the goal of optimizing the oscillator performance.

Figure 1 (a) shows the schematic illustration of the sample geometry. The devices are made from the multilayer structure [Co 0.5/Pt 2]/Co 0.6/Cu 2/Co 4/Cu 4/Co 4/Cu 2/[Co 0.2/Ni 0.8] 8 (the number after each element is the film thickness in nm), along with buffer layers and capping layers. The films are deposited using magnetron sputtering on a thermally oxidized Si wafer with a base pressure 10⁻⁹ Torr. Nanofabrication is performed to pattern the film into elliptical shape by electron-beam lithography and an Ar ion milling technique. The lateral cross section, a 170 x 130 nm² ellipse, was measured by a scanning electron microscope before the top electrode deposition (Figure 1(b)). Magnetization measurements on the unpatterned film reveal that the Co/Pt and Co/Ni multilayers have their magnetic moments oriented perpendicular to the sample plane while the two individual Co layers (the “free layers”) are oriented in-plane.

When a DC bias is applied to these devices, spin transfer torque from the spin polarized current flowing perpendicular to the layers generates precession of the magnetic moments in the system, which results in an increased magnetic moment. The precession produces a microwave output signal, whose properties vary as a function of the current bias and the external magnetic field (Figure 2). We observed microwave oscillations for both directions of applied current, with linewidths as narrow as 74 MHz. The current dependence of the oscillation frequency is not consistent with the simplest macrospin model, in which one would expect the magnetizations of the free layers to precess around an out-of-plane axis. Rather, micromagnetic simulations show that spatial inhomogeneities in the magnetic dynamics are essential in understanding the output signals. The persistent magnetization oscillations in this device geometry originate from the nucleation
and the propagation of domain walls moving back and forth within the cross-sectional area of each free layer. The dynamical motions of the domains within the two free layers are synchronized via magnetostatic coupling and spin-transfer torque between the layers, as shown in Figure 3. The oscillation mechanisms observed in this device geometry are promising for future development of spintronic oscillators, in that they combine operation at zero external magnetic field, frequency doubling (the oscillation frequency of the magnetoresistance is double the natural oscillation frequency of the magnetization), and a reduced linewidth due to phase locking between the two magnetic free layers.

References:

Plasmon Resonance in Individual Nanogap Electrodes Studied Using Graphene Nanoconstrictions as Photodetectors

CNF Project # 598-96
Principal Investigator(s): Daniel C. Ralph, Paul McEuen
User(s): Sufei Shi, Xiaodong Xu

Affiliation(s): Physics Department, Cornell University
Primary Research Funding: NSF/DMR, NSF/CCI
Contact: ralph@ccmr.cornell.edu
Web Site: http://people.ccmr.cornell.edu/~ralph

Abstract:
We achieve direct electrical read-out of the wavelength and polarization dependence of the plasmon resonance in individual gold nanogap antennas by positioning a graphene nanoconstriction within the gap as a localized photo-detector [3]. The polarization sensitivities can be as large as 99%, while the plasmon-induced photocurrent enhancement is 2-100. The plasmon peak frequency, polarization sensitivity, and photocurrent enhancement all vary between devices, indicating the degree to which the plasmon resonance is sensitive to nanometer-scale irregularities.

Summary of Research:
We grow single-layer graphene on copper foil using CVD in a furnace [1]. After spin-coating a thick PMMA layer onto the graphene, we wet etch to dissolve the copper foil completely and transfer the graphene to a highly n-doped Si substrate with 300 nm thermal oxide on top. We confirm that the graphene is mostly single layer by optical imaging and Raman spectroscopy. We then define multiple Ti/Au contacts by photolithography. Electron beam lithography is used to define the critical feature, a gold nanowire ~100 nm wide. A highly n-doped silicon substrate is used as a back gate.

We apply two steps of an electromigration technique to make a graphene nanoconstriction coupled to a sub-10 nm gold break junction. In the first step, we use electromigration with electronic feedback [2] at room temperature in air to break the Au wire and leave a nanoscale gap that will correspond to the high-electric-field region of the plasmonic antenna. The graphene layer under the gold is unaffected by this step. We then narrow the graphene wire into a nanoconstriction without breaking it fully using a second stage of electromigration in vacuum. Because graphene nanoribbons can sustain much higher current density than Au, this requires much larger voltages, 2-5 V, consistent with previous reports. Figure 1 shows an SEM image of the final device.

We perform scanning photocurrent (PC) measurements using a Ti-sapphire tunable continuous wave laser source focused to a 1.2 μm spot size with incident power ranging from 1 μW to 1 mW. We measure the PC and the reflected light simultaneously as we scan the position of the laser spot. Correlation between the reflection image and PC...
image (Figure 2) shows that a symmetric-in-position PC response arises from the narrowest region of the breakjunction device, to within the resolution of the laser spot size. A separate antisymmetric-in-position PC signal can also arise due to heating in the electrodes.

The amplitude of the symmetric PC signals for the narrow graphene nanoconstrictions varies strongly as a function of the wavelength and polarization of the incoming light. Figure 3 shows the wavelength response of the PC for a ~ 5 MΩ contact at room temperature. The PC is sharply peaked at 790 nm, typical for the plasmon resonance of an Au nanostructure, with a full width at half maximum of 40 nm. Figure 4 shows the dependence of the PC on the polarization of the incoming light for a different (R = 80 kΩ) device. The PC varies strongly with the polarization angle in a simple dipole pattern, with a factor of 11 variation from minimum to maximum response. The wavelength and polarization dependence studies show that the PC signal arises from the plasmon resonance of the gold nanogap electrode. The resonance properties vary from device to device, demonstrating the importance of geometrical variations in the performance of optical antennas at the nanometer scale.

References:

Making an Electric-Field-Controlled Giant Magnetoresistance Device Using Multiferroic Material

CNF Project # 598-96
Principal Investigator(s): Daniel C. Ralph
User(s): Chen Wang

Affiliation(s): Department of Physics, Cornell University
Primary Research Funding: ARO/MURI, NSF/DMR and NSF/NSEC
Contact: ralph@ccmr.cornell.edu, cw328@cornell.edu

Abstract:

We make giant magnetoresistance (GMR) magnetic multilayer devices (NiFe/Cu/NiFe) on top of BiFeO$_3$ films that are simultaneously ferroelectric and antiferromagnetic. We observe an exchange-bias pinning on the bottom magnetic layer of the multilayer due to interaction with BiFeO$_3$, which can be altered by an electric field applied to the BiFeO$_3$ and is partially reversible by reversing the field. We are working to use control over the exchange bias to achieve electric-field-driven manipulation of the magnetization direction of the bottom NiFe magnetic layer.

Summary of Research:

Bismuth ferrite (BiFeO$_3$) is the only known room-temperature multiferroic material showing both ferroelectric and antiferromagnetic order. Because the two order parameters are intrinsically coupled to each other, it has been shown that an applied electric field that switches the electric polarization of a BiFeO$_3$ domain will switch the antiferromagnetic order parameter as well [1]. It has also been observed that BiFeO$_3$ can produce an exchange bias pinning field on an adjacent magnetic film, and this exchange bias field can be switched together with the antiferromagnetic order parameter [2]. This presents a possibility that we can make a magnetic storage device controlled entirely by an applied electric field, with negligible power consumption.

We grow BiFeO$_3$ films of 50-100 nm on top of SrTiO$_3$, DyScO$_3$, or TbScO$_3$ substrates by pulsed laser deposition or molecular beam epitaxy, and then transfer the substrates into a sputtering chamber after a brief sonication cleaning with acetone/IPA solvent. We sputter a multilayer stack (from bottom to top) of Py (2.5 nm) / Cu (4-8 nm) / Py (2.5 nm) / Pt (2.5 nm) [where Py is permalloy = Ni$_{81}$Fe$_{19}$] onto the BiFeO$_3$ surface in a 200 Oe magnetic field, and then etch the metallic layers into either micron-scale (50 µm × 2 µm) or nano-scale (80 nm × 5 µm) devices by ion milling. The former pattern is done by photolithography and the latter is done by electron-beam lithography.

We put copper contacts on both ends of the stripe-shaped devices for current-in-plane electrical measurements. Most device stripes are designed to be tilted 45° away from the exchange bias direction but other angles were also attempted. We also deposit Cu electrodes 1.5-2 µm away and along both sidelines of the device stripe using photolithography and ion beam deposition. This pair of electrodes is used to apply an electric field across the area of BiFeO$_3$ that provides exchange bias pinning under the magnetic stripes (Figure 1).

We choose permalloy (Py) as our magnetic material because its magnetization direction can be switched easily relative to other magnets. We observe exchange bias pinning between...
Py and BiFeO$_3$ that usually exceeds the coercive field of the Py film on BiFeO$_3$, and can sometimes be as large as 90 Oe for the 2.5 nm Py film. Our resistance measurements on the devices exhibit the current-in-plane giant magnetoresistance effect, and the exchange bias is demonstrated by a shift of the magnetic hysteresis loop corresponding to the bottom Py layer pinned by BiFeO$_3$ (Figure 2).

An applied electric field can switch the net in-plane polarization of the ferroelectric BiFeO$_3$ by 90°, and the exchange bias direction is expected to be switched by 90° as well (as shown in Figure 1) so that its projection along the device stripe is reversed. Since the coercive field of the magnetic layer is smaller than the magnitude of exchange bias (as shown in Figure 2), such a switching of exchange bias can principle drive switching of the pinned layer magnetization direction near zero applied magnetic field. We have applied voltages on BiFeO$_3$ up to 140-200 V in 20 ms pulses on the 4-6 µm electrode spacing, producing electric fields larger than typical electric polarization coercivity of the BiFeO$_3$ on these substrates. However, thus far we have not observed full reversal of the exchange bias. Instead in some samples we find that the exchange bias is altered by an applied electric field in a partially reversible fashion. Electric field in one direction can reduce the exchange bias, while a reversed electric field can produce a partial restoration (Figure 3), but after repeated electric poling the exchange bias eventually decreases and saturates to a small value.

Piezo-force microscopy studies of our devices show that the domain structures of the BiFeO$_3$ between the device and one of the side electrodes change after the electric field has been applied, in the sense that the direction of the domain walls has rotated by 90° (Figure 4). This is consistent with the domain structure changes in previous studies and with the expected 90° switch of the net in-plane polarization. However, we also note that after back-and-forth poling the domain size becomes much larger and more spatially-varied than in its pristine state, indicating some irreversibility of the complex multi-domain ferroelectric ordering. The origin of exchange bias between BiFeO$_3$ and a ferromagnetic metal is also still an open question, but some inverse correlation between the ferroelectric domain size and exchange bias has been established in the case of CoFe [3]. In future work we will use nano-scale devices to study the exchange pinning within a single domain of BiFeO$_3$, so as to greatly reduce the complexity associated with the changing domain structures.

References:
Dissipation in Ultrathin Membranes

CNF Project # 762-99
Principal Investigator(s): Harold G. Craighead, Jeevak M. Parpia
User(s): Vivekananda P. Adiga

Affiliation(s): Applied and Engineering Physics, Cornell University
Primary Research Funding: NSF
Contact: hgc1@cornell.edu, vpa8@cornell.edu
Web Site: http://www.hgc.cornell.edu/

Abstract:

Stoichiometric amorphous high tensile stress SiN resonators have shown extremely a high quality factor $Q$ (> 1,000,000) at room temperature. We have fabricated large (up to 400 µm diameter) high tensile stress (~ 1.2 GPa) circular SiN membranes using both optical lithography and measured the resonant frequency and $Q$ using optical interferometric detection. The observed mechanical $Q$ shows a strong modal dependence, indicating the influence of clamping losses [2]. These findings pave the way for identifying optimum high $Q$ modes of tensioned oscillators for applications in mass sensing and optomechanical coupling experiments.

Summary of Research:

Mechanical resonators are useful for applications in high frequency devices such as filter, oscillators and sensing applications. Important parameter that determines the applicability of these devices is the quality factor in these resonators. High tensile stress silicon nitride membranes have exceptionally high quality factors and therefore are useful for such device applications. High tensile stress silicon nitride membranes show a quality factor which is two orders of magnitude higher than that of other amorphous materials at low temperature showing a departure from universality observed in glasses and other disordered materials [1]. Understanding the physical origins of dissipation are important in achieving resonators with high quality factors.

Stoichiometric tensile (1.2 GPa) silicon nitride films (110 nm) are grown on top of oxide/silicon substrate. We fabricated optically defined silicon nitride circular resonators (50 µm to 400 µm in diameter) with etch release holes (1 µm diameter) which are 5 µm apart on silicon dioxide/silicon. Resonators are released in BOE followed by critical point drying as shown in Figure 1. Resonance and dissipation in these resonators are measured by optical interferometric technique under vacuum (< 1 × 10^-6 torr).

Quality factors of the resonators show a strong modal dependence wherein azimuthal harmonics of large circular resonators (diameter > 200 µm) show an exponential drop in dissipation within an individual modal family (n = 1,2,3..., m) due to the destructive interference between the waves radiated by adjacent sections of periphery [2]. Higher order modes of large resonators and modes of smaller resonators are dominated by a characteristic fQ limit of $5 \times 10^{12}$ possibly indicating the presence of intrinsic dissipation in the high frequency limit (Figure 2).

Results are useful in finding the optimum modes for experiments involving optomechanical coupling, sensing experiments. Future work includes temperature dependent measurements of dissipation in these devices.

Acknowledgements:

We appreciate the research collaboration with Rob Ilic.
V.P.A. is supported by an NSF grant.

References:

Figure 1: Optical image of a 400 µm drum resonator fabricated using conventional optical lithography. Thickness of the membrane resonator is ~ 15 nm.

Figure 2: Modal dependence \( nx, m = 1, \) where \( n = 0,1,2,.. \) of membrane resonators of different diameters indicating the presence of a \( fQ \) limit.
Vortex Dynamics in Nanofabricated Superconducting Devices

CNF Project # 1314-05
Principal Investigator(s): Britton L.T. Plourde
User(s): Ibrahim Nsanzineza

Affiliation(s): Department of Physics, Syracuse University
Primary Research Funding: National Science Foundation; NSF-DMR-0547147
Contact: bplourde@phy.syr.edu, insanzin@syr.edu
Web Site: http://www.phy.syr.edu/~bplourde

Abstract:

We are fabricating superconducting devices for controlling the dynamics of vortices with experiments ranging from dc measurements up to microwave frequencies. Vortices are quantized bundles of magnetic flux that thread many different superconductors over a particular range of applied magnetic field. These measurements are useful for probing fundamental physical properties of vortices and for developing devices based on the controlled motion of magnetic flux in superconductors, including vortex ratchets. In addition, trapped vortices are an important loss mechanism that can limit the performance of superconducting microwave detectors and quantum coherent circuits.

Summary of Research:

For technological applications of superconductors in large magnetic fields, controlling the dynamics of magnetic flux vortices that penetrate the superconductors is important, as the motion of many vortices can cause unwanted dissipation. The addition of defects to the superconductor can pin the vortices in place and hinder their motion. In this case, each vortex can be treated as a classical particle interacting with a potential energy landscape generated by the pinning defects and the other vortices. By nanofabricating pinning structures, it is possible to control the vortex dynamics to probe such phenomena as commensurability and ratchet effects [1]. Nanofabricated devices are also useful for probing the microwave response of vortices in superconductors. Vortices trapped in superconducting traces can result in substantial reductions in the quality factor of microwave resonators. Thus, understanding and controlling this dissipation mechanism can be important in the design of superconducting systems that use microwave resonators, including sensitive photon detectors and quantum computing applications.

We are fabricating a system of superconducting, thin-film microwave resonators for studying the loss contributed by trapped flux over the frequency range from 2-11 GHz [2]. By cooling the resonators in different magnetic fields, we are able to probe the loss from vortices as a function of field at the resonance frequencies contained in our design. For some resonators, we have also been exploring the addition of nanostructured vortex pinning with a corresponding reduction in the loss due to trapped flux by over an order of magnitude compared to resonators without such patterned pinning [3].

Following a technique developed at Leiden University for controlling vortex confinement [4], we fabricate devices with narrow thin-film channels with weak vortex pinning

Figure 1: Optical micrograph of coplanar waveguide Al microwave resonator on sapphire substrate.
surrounded by banks of different superconductor with much stronger pinning. Such a structure allows easy motion of vortices in the weak-pinning channels, while the vortices in the strong-pinning banks remain immobilized. In our research program, we are fabricating similar weak-pinning channels but with various constrictions of the channel walls for controlling the potential energy landscape experienced by vortices in the channels. We have recently been studying commensurability and hysteresis in periodic sub-micron channel constriction structures [5].

We fabricate our microwave resonators from various superconducting films, including aluminum deposited onto sapphire or silicon wafers in our electron-beam evaporator at Syracuse University. We define the patterns on the Autostep 200 and transfer them into the films with reactive ion etching. We measure these circuits at temperatures down to 300 mK in our lab at Syracuse University. We fabricate our weak-pinning channels from bilayer films deposited at Leiden University. The lower weak-pinning film consists of an amorphous layer of NbGe, while the upper film is a 50nm-thick layer of reactively sputtered NbN, which has strong pinning. We produce channels as narrow as 150 nm with electron-beam lithography and reactive ion etching using CF4. We measure these channel devices in cryogenic systems that we have constructed in our lab at Syracuse University.

References:


Melting Dynamics of Colloidal Crystals on Patterned Surfaces

CNF Project # 1361-05
Principal Investigator(s): Itai Cohen
User(s): John Mergo, John Savage

Affiliation(s): Laboratory of Atomic and Solid State Physics, Department of Physics, School of Applied and Engineering Physics; Cornell University
Primary Research Funding: King Abdullah University of Science and Technology (KAUST)
Contact: itai.cohen@cornell.edu, jcm387@cornell.edu, jrs423@cornell.edu
Web Site: http://cohengroup.ccmr.cornell.edu

Abstract:

The melting dynamics of colloidal crystals are studied in the presence of patterned substrates created using electron-beam lithography. Patterned substrates allow for the control of surface symmetry and lattice constant in an otherwise “hard-sphere” system. Crystalline islands are self-assembled on the patterned substrates and then melted. The underlying substrate symmetry and strain are found to alter both growth and melting dynamics, including the diffusion of adatoms on growing islands, sub-diffusion in lattice interstitials, and the melting rate of individual islands.

Summary of Research:

Microfabricated templates have been successfully used to direct the growth of colloidal particles into self-assembled structures [1]. This technique allows for accelerated colloidal crystallization, which has been exploited to study the effects of various boundary conditions, including stretched templates [2] and surfaces with embedded grain boundaries [3]. Recently we have used this technique to report the diffusive nature of step-edge barriers and island growth in epitaxially grown colloidal crystals [4].

In our current research project, we construct a 10,000 sq. micron grid consisting of 1.0 µm holes placed 500 nm deep into glass. A mixture of 1.0 µm charge-stabilized polystyrene colloidal particles and a nonionic surfactant is sedimented onto the patterned surface. The holes trap a monolayer of particles, forcing them to assume the underlying symmetry, while the surfactant serves to introduce an attractive force between the colloids. A single crystalline layer directly above the trapped layer is studied using an inverted microscope. The dynamics of crystallization of this layer of colloidal particles is directly observed with single particle resolution in real time.

Substrate fabrication utilizes electron-beam lithography to pattern periodic arrays of 1.0 µm holes in a 500 nm thick layer of polymethylmethacrylate (PMMA) with a center-to-center distance of 1.05 µm (Figure 1). This pattern is transferred into the glass via a chromium mask and reactive ion etch. A square lattice of micron-size holes is used to grow a face-centered cubic crystal along the <100> face, while a triangular lattice can be used to explore the <111> face. In combination with a temperature dependent attractive interaction [5], we are able to observe the dynamics of both island growth and melting. An initial layer of colloidal particles self-assemble into the holes due to the surfactant-induced attraction between particles and between particles and the substrate (Figure 2). Island growth occurs atop the initial layer of colloidal particles with the same symmetry as the underlying lattice. A small change in temperature allows us to weaken the attractive forces in the system, causing the islands to melt. Because of the geometric constraints that the lattice imposes on the diffusion of particles, the rate of melting is found to vary dramatically depending on the underlying lattice symmetry (Figure 4).

References:

Figure 1: SEM of 1.0 µm holes written into PMMA on a glass cover-slip patterning using electron-beam lithography. The features between the holes are unexposed PMMA with a width of 50 nm. The upper-left corner of the image displays the FCC [111] (triangular) configuration of holes, while the lower-right corner features the FCC[100] (square) array.

Figure 2: Optical image of the self-assembly of two layers of 1.0 µm polystyrene particles on a triangularly patterned substrate. The white (in-focus) particles are particles that reside on the second layer of this crystal, which are diffusing atop the lattice of black (out-of-focus) particles. The black particles reside in the holes in the patterned substrate shown in Figure 1. The patterned holes are visible on the top-left and bottom corners of the figure, and appear as a faint “third layer.”

Figure 3: Plots of island size versus time for colloidal particles crystallized on a patterned substrate. Comparisons between lattice symmetries show that the melting rate on a square face is about three times slower than that on a triangular face.
Microfluidic Chambers for Studies of Confined Superfluid He-3

CNF Project # 1520-07
Principal Investigator(s): Jeevak Parpia
User(s): Robert Bennett, Nikolay Zhelev

Affiliation(s): Laboratory of Atomic and Solid State Physics, Cornell University
Primary Research Funding: National Science Foundation
Contact: jeevak@ccmr.cornell.edu, rgb77@cornell.edu

Abstract:

We have studied superfluid $^3$He confined to submicron slab geometries inside nanofabricated, microfluidic chambers. Two separate techniques were used; nuclear magnetic resonance (NMR) and the torsional oscillator (TO). NMR studies have shown a significant modification to the superfluid $^3$He phase diagram as a result of the confinement. However, the NMR sample chamber suffers from significant distortion under increasing pressure. The TO studies have observed a decoupling of the $^3$He in the normal state, thus preventing study of the superfluid state so far. Our current work has been focused on fabricating new NMR and TO cells to overcome their respective problems.

Summary of Research:

The order parameter of superfluid $^3$He is suppressed at a boundary and recovers over a length scale on the order of the coherence length, $\xi$. The coherence length is pressure and temperature dependent, varying from 78 nm to ~15 nm between 0.0 and 34 bar at $T = 0.0$. When a sample of superfluid $^3$He is confined to a slab geometry, of thickness on the order of $\xi$, the phase diagram is predicted to be modified from that of bulk liquid, and previously unobserved order parameters may also be stabilized [1].

Our original NMR cell consisted of a 10 mm \(\times\) 7 mm rectangular chamber and the TO cell consisted of a 10 mm outer diameter, 4 mm inner diameter circular chamber [2]. The chamber height for both cells was $d = 640$ nm ($d/\xi \approx 8.3$ at $p = 0$, $T = 0$). The chambers were etched into a 3 mm thick piece of silicon and then sealed by anodic bonding of a 3 mm thick piece of Hoya SD-2 glass to the silicon. Thick pieces of silicon and glass were used to allow pressure tuning of the effective confinement, $d/\xi$, while minimizing distortion of the cells.

The NMR experiments, carried out at Royal Holloway University, revealed a significant modification of the bulk phase diagram [3] and a hysteretic transition to an unidentified superfluid phase was also observed [4]. However, despite the use of the 3 mm thick silicon and glass, subsequent optical characterization of the NMR cell revealed significant distortion under pressure, on the order of 25 nm/bar at the center of the cell. Therefore a new cell design is required in order to reduce the cell distortion under pressure.

Increasing the thickness of the silicon and glass is not an option, since this will reduce the filling factor of the $^3$He sample inside the NMR receiver coil. Therefore a supporting structure is required to...
reduce the distortion. The new design (see Figure 1) includes a 1 mm thick wall down the center of the cell, to which the glass will also be bonded. The chamber height of the new cells will also be increased to 1 µm, so as to increase $d/ξ$ at zero pressure and place us closer to the domain of a new superfluid phase that is predicted to exhibit broken translational symmetry [1].

The TO experiments, carried out at Cornell, observed complete decoupling of the normal $^3$He from the oscillator below 100 mK [5], thus preventing a study of the superfluid state. Based on scans of the glass and silicon by atomic force microscopy (see Figure 2) and the analysis [6] of similar observations in a silver TO cell, we believe that the decoupling of the normal fluid was a result of the very low surface roughness of the silicon and glass.

Therefore we are currently working on producing new TO cells in which the silicon surface is controllably roughened. The method we are using involves evaporating a very thin film (nominally 1-2 nm) of gold onto the silicon. Such a film is not continuous, but instead consists of many small islands of gold, tens of nm in diameter. The gold islands can then be used as a mask for a reactive ion etch (RIE), thus patterning the silicon with an array of tiny nanopillars. Following the RIE, the gold is removed by wet etching.

Figure 3 shows a silicon surface patterned with a nominally 1.2 nm thick gold film and then etched with CF$_4$ plasma. The diameters of the gold islands range from about 10 to 40 nm and the etch depth (i.e. pillar height) was measured to be 11 nm by placing a witness sample inside the etcher. Calculations by Priya Sharma at Royal Holloway, have shown that such a surface should keep the normal fluid locked to the oscillator well below the superfluid transition, thus enabling a study of the superfluid state.

Distortion of the TO cells is not such a concern, since the width of the un-bonded area is much less than that of the NMR cell, but the chamber height of the new TO cells has also been increased to 1 µm for the same reason as described above for the NMR cells.

References:


Figure 2: Atomic force micrograph of the glass surface. Fits to the height distribution data and the surface autocorrelation function give a surface roughness of 0.85 nm and a correlation length of 73 nm.

Figure 3: Scanning electron micrograph of a silicon surface patterned as described in the text. The image was taken before the gold was removed to improve contrast.
Persistent Currents in Normal Metal Rings

CNF Project # 1527-07
Principal Investigator(s): Jack Harris
User(s): Manuel Angel Castellanos Beltran, William Ennis Shanks

Affiliation(s): Physics and Applied Physics, Yale University
Primary Research Funding: National Science Foundation, Division of Materials Research; Yale University
Contact: jack.harris@yale.edu, manuel.castellanosbeltran@yale.edu, will.shanks@yale.edu
Web Site: http://www.yale.edu/harrislab

Abstract:
Measurements of persistent currents in diffusive metal rings can be used to test the validity of the theory that explains electronic diffusion in metallic systems. The value of these currents is a stochastic function of the disorder profile, and thus different from sample to sample. Our test consists of studying the distribution function of the measured persistent currents. In order to probe the underlying distribution of the stochastic function we need to study the statistics of many independent samples. We do so by measuring eight different samples over a large magnetic field range.

Summary of Research:
A remarkable prediction of mesoscopic physics is that a resistive metal ring can support a dissipationless electrical current [1]. This persistent current (PC) is quantum in nature and is analogous to the net orbital angular momentum of the electrons orbiting some atoms. In order for this persistent current to be appreciable, though, the circumference of the ring must be smaller than both the electron phase coherence length in the metal and the thermal length, both of which are on the micron size scale for millikelvin temperatures. Another crucial point is that in order to observe all this motion happening within the ring, we need to break time-reversal symmetry by applying a magnetic flux through the ring. This results in stationary flux-dependent circulating current with periodicity of flux quantum \( \hbar/e \) with \( \hbar \) being Planck’s constant and \( e \) the electron charge.

The order of magnitude of the PC for our rings is of the order of 1 nA. Although a current of 1 nA is not technically hard to measure, the experimental difficulty arises from the fact that the PC flows only within the ring and so it can only be measured by non-invasive methods. Our group has recently showed that torsional magnetometry can be used to measure PC with an excellent sensitivity [2]. Our approach consists of fabricating ultra-sensitive cantilevers integrated with single metal rings. An SEM picture of a characteristic sample is shown in Figure 1. When a current flows in the ring, its magnetic dipole moment couples to the mechanical motion of the cantilever. This makes the resonance frequency of the cantilever a function of the current in the ring. We monitor the cantilever resonance frequency using laser interferometry as we sweep the magnetic field. The sensitivity compared to previous measurements was increased to 0.2 nA/√Hz for a ring with 2 µm circumference at 9 T.

One important point about the PCs in our rings is that, like many mesoscopic effects in disordered systems, they depend on the particular realization of disorder and thus vary between nominally macroscopically identical systems.

Figure 1: Electron micrograph of the experimental device. Several Si cantilevers similar to those used in the experiment are shown in the main picture. An individual ring is shown in the inset.
Theory has predicted the persistent current to be a random variable whose ensemble average vanishes and have a particular typical magnitude (or second cumulant) already studied by our group in previous measurements\cite{2}. Theory also predicts that for metallic rings all of the other higher cumulants vanish, and thus we expect the distribution function to be Gaussian \cite{3}. Our new measurements tested this prediction.

The inset of Figure 2 contains a representative plot of measured persistent current versus magnetic field, showing its characteristic periodicity in applied field. As observed in Figure 2, the persistent current oscillation also has a finite correlation (shown as an aperiodic modulation of the amplitude) in applied magnetic field due to the field penetrating the metal \cite{4}. This implies that distant magnetic field points give statistically independent measurements of the current magnitude. Thus, the expected magnetic dependence of the measured PCs is given approximately by the following equation:

\[
I(B_m,\phi) = I^+(B_m)\cos\left(2\pi\frac{\phi}{\phi_0}\right) + I^-(B_m)\sin\left(2\pi\frac{\phi}{\phi_0}\right)
\]

where the variables \(I^+\) and \(I^-\) are stochastic variables that vary with the magnetic field \(B_m\). These are shown in the main plot of Figure 2. Our goal is determining whether the distribution of \(I^+\) and \(I^-\) agrees with the predictions done so far that they are Gaussian.

This finite correlation also allows us to effectively take a large number of independent measurements by sweeping the magnetic field over a large range. We performed measurements over seven more samples on top of a single ring measured in previous measurements. The consolidated data of our measurements is shown in Figure 3. The estimates of the measured first six cumulants agree with the expected values within the statistical and experimental error, thus confirming that the measured distribution of the amplitude of the persistent currents is Gaussian.

References:

\begin{enumerate}
\end{enumerate}
Quantum-Limited Measurement and Entanglement in Superconducting Circuits

CNF Project # 1577-07
Principal Investigator(s): Robert McDermott
User(s): Remote Project

Affiliation(s): Department of Physics, University of Wisconsin-Madison
Primary Research Funding: Intelligence Advanced Research Projects Activity (IARPA)
Contact: rfmcdermott@wisc.edu

Abstract:

We are developing novel quantum-limited detection tools for the characterization of entanglement in circuits comprising superconducting quantum bits (“qubits”) and linear thin-film microwave resonators. We have realized a detector of single microwave photons based on the current-biased Josephson junction. The design is readily scalable to tens of parallelized detection channels, a configuration that will allow number-resolved counting of microwave photons. In addition, we have developed a novel low-noise microwave amplifier based on the Superconducting Low-inductance Undulatory Galvanometer (SLUG). The device should achieve noise performance approaching the standard quantum limit in the frequency range from 5-10 GHz.

Summary of Research:

We are developing two classes of novel quantum-limited detection tools for the study of entanglement in systems comprising superconducting qubits and microwave thin-film cavity resonators.

First, we are developing a novel microwave counter based on the Josephson junction. The junction is tuned to absorb single microwave photons from the incident field, after which it readily tunnels into a classically observable voltage state. Using two such detectors, we have performed a coincidence counting version of the Hanbury Brown and Twiss experiment at 4 GHz and demonstrated a clear signature of photon bunching for a thermal source. The design is readily scalable to tens of parallelized junctions, a configuration that would allow number-resolved counting of microwave photons for state reconstruction or for studies of the full counting statistics of microwave noise emitted by mesoscopic conductors. In addition, we are developing microwave amplifiers based on the Superconducting Low-inductance Undulatory Galvanometer (SLUG). The low-inductance gain element is integrated into a microwave thin-film resonator, providing for efficient coupling of a microwave-frequency signal to the SLUG. Gain in excess of 20 dB has been demonstrated at frequencies over 8 GHz, with bandwidth of order 100 MHz. System noise temperatures of 1 K have been measured; the amplifier noise is currently limited by hot electron effects. We expect that optimized devices should achieve noise performance approaching the standard quantum limit for linear phase-insensitive amplifiers.

We have used the CNF to fabricate reticles that are needed for the preparation of thin-film superconducting devices at the Wisconsin Center for Applied Microelectronics (WCAM). Superconducting aluminum and niobium thin films are grown by sputter deposition, while dielectric films are grown by plasma-enhanced chemical vapor deposition. The films are patterned photolithographically and etched with chlorine- and fluorine-based reactive ion etching. Device characterization is performed at millikelvin temperatures in our laboratories at the University of Wisconsin.
Figure 1: Multiplexed microwave photon counter sample comprising two fluxed-biased Josephson junctions coupled to a single microwave cavity.

Figure 2: Superconducting Low-inductance Undulatory Galvanometer (SLUG) gain element used in ultralow-noise microwave amplifier.
Magnetic Tunnel Junction Based Orthogonal Spin Transfer Devices

CNF Project # 1673-08
Principal Investigator(s): Andrew D. Kent
User(s): Dirk Backes, Pradeep Manandhar, Salil Nanda

Affiliation(s): Department of Physics, New York University
Primary Research Funding: Spin Transfer Technologies, LLC
Contact: adk1@nyu.edu, db146@nyu.edu, pradeep.manandhar@spintransfer.com, salil.nanda@spintransfer.com
Web Site: http://www.physics.nyu.edu/kentlab/

Abstract:

Orthogonal spin-transfer magnetic random access memory (OST-MRAM) uses a spin-polarizing layer magnetized perpendicular to a free magnetic layer to achieve large spin-transfer torques and ultrafast energy efficient switching. We have fabricated and studied OST-MRAM devices that incorporate a perpendicularly magnetized spin-polarizing layer and a magnetic tunnel junction, which consists of an in-plane magnetized free layer and synthetic antiferromagnetic reference layer. Reliable switching is observed at room temperature with 0.7 V amplitude pulses of 500 ps duration and requires energy of less than 450 fJ.

Project Summary:

Spin-transfer torque random access memory (STT-MRAM) devices are promising candidates for a universal memory [1]. STT-MRAM is nonvolatile, has a small cell size and high endurance. Conventional collinear magnetized devices have the disadvantage of long mean switching times and broad switching distributions [2]. By employing a spin-polarizing layer magnetized perpendicular to a free layer (Figure 1), large initial spin-transfer torques can be achieved increasing the switching speed and reducing the switching time distributions [3]. We are fabricating and studying magnetic tunnel junction (MTJ) based spin transfer MRAM (OST-MRAM) devices that have the potential for sub-nanosecond switching times and large (> 100%) magnetoresistance [4], both of which are critical for applications as well as interesting for fundamental studies of spin-torque driven magnetization dynamics.

The OST-MRAM layer stack was grown on 150 mm oxidized silicon wafers using a Singulus TIMARIS physical vapor deposition module. The polarizer consists of a Co/Pd multilayer exchange coupled to a Co/Ni multilayer. The MTJ structure consists of a CoFeB/MgO/CoFeB/Ru/CoFe/PtMn magnetic tunnel junction.

The layer stacks were characterized by vibrating sample magnetometry (VSM), ferromagnetic resonance (FMR) spectroscopy, and current-in-plane tunneling measurements. Figure 2 shows VSM measurements of the film magnetization for in-plane and perpendicular-to-the-plane applied fields. The CoFeB layers are very soft while the CoFe layer

Figure 1: OST-MRAM layer stack. A perpendicularly magnetized polarizer (P) is separated by a nonmagnetic metal from the free magnetic layer (FL). The free layer forms one electrode of a MTJ. The other electrode, the reference layer, consists of a synthetic antiferromagnetic (SAF).

Figure 2: VSM measurements of the magnetization of the layer stack. The curve connecting the solid circular data points shows the switching of the FL and SAF under an in-plane applied field. The curve with square data points shows the characteristics of the polarizing layer in a field applied perpendicular to the plane, demonstrating a high remanence and a coercive field of 26 mT.
which is coupled to the antiferromagnetic PtMn has a coercive field of about 50 mT. The shift of hysteresis due to the exchange bias effect is 100 mT. The coercivity of the perpendicular polarizer is 26 mT. These films are patterned into nanopillars that are on the order of $50 \times 100$ nm$^2$ using combinations of electron beam lithography and ion-milling. In the resulting devices current flows perpendicular to the layer planes, i.e. there are top and bottom electrical contacts to the nanopillar.

Figure 3 shows device resistance versus in-plane magnetic field. From the resistance change due to the switching of the magnetic direction of the free layer we find a magnetoresistance (MR) of 107%. By applying short voltage pulses and determining the device resistance before and after the pulse we measure the switching probability. We observed 100% switching probability for pulses as short as 500 ps with an amplitude of 0.7 V at room temperature. From this we conclude that there is no incubation delay of several nanoseconds as observed in conventional collinearly magnetized devices [2]. The energy required for switching is very low, less than 450 fJ.

We are using these experimental results to optimize device characteristics by varying the device shape and layer composition. Microscopy of a device fabricated at CNF can be seen in Figure 4.

References:

Abstract:

The electrical conductivity of organic thin film devices are very sensitive to small applied magnetic fields, producing phenomena such as organic magnetoresistance (OMAR) and magnetoluminescence [1,2]. We have studied the effect of the inhomogeneous magnetic fields from a thin ferromagnetic electrode on OMAR by fabricating a device we denote a semi-spin-valve. Our device provides a means to control the electrical conductivity of an organic film at room temperature, using the spatially-varying magnetic fringe fields from a magnetically-unsaturated ferromagnet.

Project Summary:

We have fabricated an organic semiconductor device consisting of a ferromagnetic layer, a hole-injecting layer (a PEDOT polymer), an organic semiconductor (Alq3), and a capping electrode (CaAl) (see Figure 1). The ferromagnetic electrode (fringe fields source) is a CoPt multilayer deposited using electron-beam evaporation in ultra high vacuum on oxidized Si wafers for device studies and Si supported Si3N4 windows for magnetic domain imaging studies using an x-ray transmission microscope. Optical lithography is used to define the bottom electrode geometry. A hole-injecting layer followed, either by sputtered indium tin oxide (ITO) or the conducting polymer poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) deposited by spin-coating from an aqueous suspension (suspension purchased from H. C. Starck, CLEVIO P VP AI 4083). A 30 nm thick film of organic semiconductor Alq3 (sublimed grade, purchased from HWSands Corp.) was deposited by thermal evaporation in high vacuum and at room temperature. A Ca (10 nm) layer was used to take advantage of the favorable work function of Ca, and was covered by a capping layer of Al (40 nm).

The properties of the ferromagnetic electrodes were characterized in detail using a variety of complementary techniques. We have used vibrating sample magnetometry (VSM) to determine the electrodes’ magnetization versus field (hysteresis loops) and correlate it with magnetotransport properties of organic semi-spin-valve devices (see Figure 2). The experiments in Figure 2 were performed in a perpendicular applied magnetic field. The electrode was also

Figure 1: Schematic plot of the semi-spin-valve: a ferromagnetic layer (CoPt), a hole-injecting layer (PEDOT), an organic semiconductor (Alq3), and a capping electrode (CaAl).

Figure 2: Correlation between magnetoconductivity in the organic devices and magnetic switching in the ferromagnetic electrodes. Upper panel shows magnetoconductivity in the organic devices, bottom panels, VSM measurements of the magnetic electrodes prior to completion of the device (i.e. unpatterned bottom electrodes).
that demonstrates that the observed magnetoresistance occurs in the organic semiconducting (Alq₃) layer independently of the nature of the bottom electrode. We claim that our magnetoconductivity effect is caused by the fringe field distribution inside the organic semiconducting layer, not by spin-polarized injection from the ferromagnetic layer into the organic semiconductor. We have built a control device that was electrically isolated from the ferromagnetic film to prove that our semi-spin-valve effect was not caused by spin injection. A thin dielectric has been deposited on the ferromagnetic film and capped with a 12 nm Pt layer. The current path is therefore entirely outside the ferromagnetic thin film (i.e., in the Pt layer), and spin-injection cannot occur, yet the same magnetoconductivity response was observed.

A typical magnetoconductivity trace for an organic device fabricated without a ferromagnetic layer (using a bottom electrode of ITO) is caused by random hyperfine fields. The hyperfine-induced magnetoconductivity response has a magnitude of several percent in our Alq₃ devices, saturates for fields in excess of 0.1 T, is non-hysteretic, and has a full-width-at-half-maximum of approximately 20 mT. Figure 2 shows a magnetoconductivity curve of a semi-spin-valve and their correlation with magnetic hysteresis loops of the ferromagnetic electrode. Magnetoconductivity (upper panel) changes are largest at the coercive field and the conductivity is suppressed between the nucleation field and saturation field of the ferromagnetic electrode.

A control device where the synthetic metal (PEDOT) bottom electrode was replaced with an inorganic metal (ITO) was measured. ITO is a commonly employed electrode material for OLEDs. We achieved a similar magnetoconductance effect comparable to the device with PEDOT-electrode — that demonstrates that the observed magnetoresistance occurs in the organic semiconducting (Alq₃) layer independently of the nature of the bottom electrode.

We claim that our magnetoconductivity effect is caused by the fringe field distribution inside the organic semiconducting layer, not by spin-polarized injection from the ferromagnetic layer into the organic semiconductor. We have built a control device that was electrically isolated from the ferromagnetic film to prove that our semi-spin-valve effect was not caused by spin injection. A thin dielectric has been deposited on the ferromagnetic film and capped with a 12 nm Pt layer. The current path is therefore entirely outside the ferromagnetic thin film (i.e., in the Pt layer), and spin-injection cannot occur, yet the same magnetoconductivity response was observed.

References:

Fabrication of Nanoscale Josephson Junctions for Quantum Coherent Superconducting Circuits

CNF Project # 1735-08
Principal Investigator(s): Britton L.T. Plourde
User(s): Pradeep Bhupathi, Michael DeFeo

Affiliation(s): Department of Physics, Syracuse University
Primary Research Funding: Defense Advanced Research Projects Agency (DARPA)
Contact: bplourde@phy.syr.edu, pbhupath@syr.edu, michael.defeo@gmail.com
Web Site: http://www.phy.syr.edu/~bplourde

Abstract:
We fabricate nanoscale superconductor tunnel junctions for experiments involving quantum coherent circuits. Such circuits have shown great promise in recent years for explorations of quantum mechanics at the scale of circuits on a chip and for forming qubits, the elements of a quantum computer. The superconducting qubit, where the entire device has two fundamental basis states, can be manipulated with microwave radiation at low temperatures. To probe such circuits, we are developing low-noise superconducting amplifiers and novel readout techniques for measuring the qubit state.

Summary of Research:
The unique properties of nanoscale Josephson junctions enable a wide range of novel superconducting circuits for investigations in many diverse areas. In recent years, circuits composed of such junctions have emerged as promising candidates for the element of a quantum computer, due to the low intrinsic dissipation from the superconducting electrodes and the possibility of scaling to many such qubits on a chip [1]. The quantum coherent properties of the circuits are measured at temperatures below 50 mK with manipulation of the qubit state through microwave excitation.

We are currently working on a variety of experiments involving these nanoscale superconducting junctions that will allow us to probe the nature of quantum entanglement between qubits and microwave photons. By incorporating these junctions into superconducting quantum interference devices (SQUIDs), we are working to develop low-noise linear amplifiers in the microwave range [2-4]. We are also fabricating lumped element superconducting oscillators for implementing novel techniques for reading out the state of a superconducting qubit [5,6].

We pattern these circuits at the CNF with nanoscale structures defined with electron-beam lithography integrated with photolithographically defined large-scale features. The junctions are fabricated using the standard double-angle...
shadow evaporation technique, in which a resist bilayer of copolymer and PMMA is used to produce a narrow PMMA air bridge suspended above the substrate. Evaporation of aluminum from two different angles with an oxidation step in between forms a small Al-AlOₓ-Al tunnel junction from the deposition shadow of the air bridge. We have developed a process for defining these junctions on the JEOL9300 and we perform the aluminum evaporations in a dedicated chamber at Syracuse. We pattern large-scale features using the Autostep 200, with electron-beam evaporation of Al and Pd films and PECVD deposition of SiO₂. Measurements of these circuits are performed in cryogenic systems at Syracuse University, including a custom dilution refrigerator for achieving temperatures of 30 mK.

References:


Carbon Nanotube p-i-n Diodes of Known Chirality

CNF Project # 1784-09
Principal Investigator(s): Robert C. Davis
User(s): Brian Davis

Affiliation(s): Department of Physics and Astronomy, Brigham Young University
Primary Research Funding: Center for Nanoscale Systems
Contact: davis@byu.edu, davis252@gmail.com

Abstract:
We fabricated electrodes for dielectrophoresis of carbon nanotubes (CNTs) on top of buried split gates [1,2] to create large arrays of carbon nanotube p-i-n diodes. We used CNTs purified to a single electronic type [3] to study diodes with known band gaps and optoelectronic properties. AFM and photocurrent spectroscopy were used to characterize the devices.

Summary of Research:
We utilized the stepper lithography system, evaporation, and lift-off to make our electrodes. Plasma enhanced chemical vapor deposition (PECVD) was used to deposit SiO2 to bury the molybdenum split gates. Cr/Au electrodes were used to perform the dielectrophoresis. The critical dimension of these electrodes was printed at less than 400 nm using the Autostep. Die-by-die alignment was used to attain the necessary alignment tolerance.

A solution of semiconducting nanotubes dispersed in an ionic surfactant was obtained through isopycnic centrifugation following Arnold et al. [3]. The wafer was rinsed vigorously in water to remove weakly adhered CNTs, and dried. Devices were imaged with atomic force microscopy (AFM) to find electrodes with single or few unbundled CNTs. Photocurrent spectroscopy was employed to study the band structure of the devices.

References:
Abstract:

Circuits based on nanoscale superconductor tunnel junctions and low-loss microwave resonators have emerged as some of the leading candidates for forming a quantum computer. The quantum coherence properties of such circuits are strongly linked to the materials properties of the various components that are used to form the devices. We are studying a variety of approaches to improving the coherence of these superconducting quantum circuits.

Summary of Research:

Superconducting circuits involving nanoscale superconductor tunnel junctions and low-loss microwave resonators are currently being investigated by many research groups worldwide for forming the elements of a quantum computer. The inherent nonlinearity of Josephson junctions allows for the possibility of forming two-state quantum systems, or qubits, and low-loss resonators provide a route for transmitting or storing single microwave quanta [1]. The ultimate performance of these circuits is tied to a variety of materials properties in the components used to form the qubits and resonators, including microwave loss and various types of noise processes [2].

We are working on a variety of approaches for probing some of the materials properties that limit the coherence of these superconducting quantum circuits. Microwave loss in the native oxide that forms on the surfaces of most superconducting thin films is one of the dominant loss channels that limits the quality factors of superconducting resonators at low temperatures [3]. We are exploring different superconducting films, including NbN, and surface treatments in an attempt to reduce the loss from surface oxides [4]. For the Josephson junctions that form the nonlinearity in most superconducting qubits, defects in the tunnel barrier and fluctuations in the critical current can limit the coherence properties of the qubit. To address the coherence problems arising from the junction barrier, we are developing a novel Josephson junction design where the junction is formed from a superconducting nanoscale constriction rather than a tunnel barrier [5].

We deposit our various superconducting films in dedicated vacuum systems, both sputtering and electron-beam evaporation, at Syracuse University. We pattern resonators from these films at the CNF with photolithography on the Autostep 200 followed by reactive ion etching. For defining the nanoscale constriction junctions, we use the JEOL 6300 to write narrow lines on a-MoGe films. We then transfer the nanowire pattern into the films by ion beam etching. We perform measurements of these circuits in cryogenic systems at Syracuse University.

References:

Figure 1: Optical micrograph of superconducting NbN coplanar waveguide microwave resonator.

Figure 2: Transmission measurement through feedline that is weakly coupled to NbN microwave resonator at 300 mK.

Figure 3: Scanning electron micrograph of 25 nm wide a-MoGe nanowire patterned by electron-beam lithography and ion beam etching.

Figure 4: Current-voltage characteristic of 25 nm wide a-MoGe nanowire measured at 1.7 K with three different frequencies of microwave irradiation.
Abstract:

We have studied the nonlinear dynamics of two superfluid $^4$He reservoirs weakly coupled through an array of nanoscale apertures. Here we summarize our recent observation of bifurcation phenomenon.

Summary of Research:

A superfluid weak link is formed with an array of nanoscale apertures (Figure 1) connecting two reservoirs of superfluid helium. Such a system exhibits macroscopic quantum behaviors that can be parameterized with a nonlinear hydrodynamic inductance associated with the weak link, shunted by a hydrodynamic capacitance arising from the presence of a diaphragm used as a pressure pump. The system constitutes a LC oscillator with the dynamics described by a phase particle in a so-called washboard potential, in analogy with superconducting Josephson junctions [1]. If such a system is driven with an ac force at a frequency slightly below the resonant frequency, a dramatic nonlinear effect should manifest itself. The system should exhibit an abrupt transition from one dynamical oscillation state to another at some critical ramping amplitude.

We have probed this nonlinear phenomenon called bifurcation in a superfluid system for the first time. We have shown that as the so-called superfluid plasma resonance is excited into a nonlinear regime, the system abruptly transitions between two dynamical states. Figure 2 shows the bending of the resonant peak towards lower frequency as well as sudden transitions from a low-amplitude and phase-lagging state to a high-amplitude and phase-leading state as the drive is increased. We have also observed bifurcation by lowering the potential well depth with temperature variations. One interesting aspect of the results obtained in this experiment is the possibility for exploiting the anharmonicity of the junction oscillator as a novel amplifier, in close analogy with rf-driven Josephson bifurcation amplifiers currently utilized in quantum computing research [2]. Further details can be found in Ref. [3].

References:

Figure 1: SEM image of aperture array. The array consists of $75 \times 75$ nominally 60 nm apertures spaced on 2 $\mu$m square lattice in a 60 nm thick silicon nitride membrane.

Figure 2: Amplitude of plasma oscillation and oscillation phase relative to the drive as a function of drive frequency.
Electronic Structure Calculations for $\text{Cr}_{1-x}\text{Al}_x$

**CNF Project # 1845-09**  
**Principal Investigator(s):** Frances Hellman  
**User(s):** Zoe Boekelheide

**Affiliation(s):** Materials Science Department, Lawrence Berkeley National Lab and Physics Department, UC Berkeley  
**Primary Research Funding:** Department of Energy  
**Contact:** fhellman@berkeley.edu, zboekelheide@berkeley.edu

**Abstract:**

$\text{Cr}_3\text{Al}$ shows semiconducting behavior that has not been explained previously. We used density functional theory calculations, performed at the Cornell NanoScale Facility to study the effect of chemical ordering and magnetism on the semiconducting behavior. The calculations show that the proposed chemically ordered $\text{Cr}_3\text{Al}$ structure in the $\text{Cr}_{1-x}\text{Al}_x$ phase diagram is the lowest energy structure of those considered. In addition, the band structure shows a pseudogap, consistent with experimentally observed transport properties. Antiferromagnetic ordering is also shown to be crucial for formation of the pseudogap. These results suggest that chemical ordering and antiferromagnetism work together to cause the unexpected semiconducting behavior in $\text{Cr}_3\text{Al}$.

**Summary of Research:**

Alloys and compounds made of metallic elements are generally expected to be metallic, and indeed most are. However, some such compounds are semiconducting or semimetallic, such as $\text{RuAl}_2$ and $\text{Fe}_2\text{VAI}$ [1]. In theory, any compound with an even number of valence electrons in the primitive unit cell can be semiconducting because the electrons can completely fill the valence band. Transition metals usually have several overlapping bands at the Fermi energy ($E_F$) so even in compounds with an even number of electrons typically several bands are partially filled. For an intermetallic compound to be semiconducting, hybridization must shift the bands in a fortuitous way, leaving a gap at $E_F$.

When intermetallic compounds do have a gap at $E_F$, they are the subject of significant study. The gap can be exploited for applications, for example, intermetallic semiconductors are attractive for thermoelectric devices due to their typically small gaps and large Seebeck coefficients (ex. ZrNiSn) [2].

In magnetic compounds, the gap is asymmetric with spin; if a gap occurs at $E_F$ for one spin but not the other, the result is a half metal (ex. $\text{Co}_3\text{MnAl}$) [3]. Half-metals are important for spintronics applications such as spin transistors and non-volatile logic.

$\text{Cr}_{1-x}\text{Al}_x$, where $x = 0.15-0.26$, shows semiconducting behavior that has not been explained until now. A maximum resistivity of 3600 $\mu\Omega\cdot\text{cm}$ occurs, with a negative temperature coefficient of resistivity [4]. A large Hall coefficient and a small electronic specific heat is observed [4,5], all hallmarks of semiconducting behavior. In addition, $\text{Cr}_{1-x}\text{Al}_x$ is antiferromagnetic for $x = 0.0-0.50$. The maximum resistivity and Hall coefficient and minimum electronic specific heat all occur around $x = 0.25$, with a plateau in the magnetic susceptibility at that point [6], suggesting an ordered compound $\text{Cr}_3\text{Al}$ is responsible for the behavior.

Our previous results included photoemission measurements showing a small semiconducting gap or pseudogap (around 95 meV) at $E_F$ in a $\text{Cr}_{0.80}\text{Al}_{0.20}$ thin film. Our density functional theoretical results showed that a disordered $\text{Cr}_{0.80}\text{Al}_{0.20}$ alloy in theory should show a pseudogap in the density of states, however the pseudogap is not as deep as expected [7]. This led us to further calculations which carefully consider the effect of possible chemical ordering and of the antiferromagnetism on the electronic structure.

DFT calculations were done on the Intel cluster at the Cornell NanoScale Facility using the AkaiKKR code, a full-potential DFT Green’s function approach based on the Korringa-Kohn-Rostoker multiple-scattering technique [8-10]. The scalar relativistic approximation was used and disorder in the bcc solid solution was treated using the coherent potential approximation (CPA) [11,12]. The generalized gradient approximation (GGA) was used to approximate the exchange-correlation energy [13].

The atoms in $\text{Cr}_3\text{Al}$ occupy the sites of a bcc lattice, like Cr. We performed density functional theoretical calculations to
compare possible types of chemical ordering and showed that the Cr$_3$Al structure proposed from TEM [14], a chemically ordered rhombohedrally distorted phase with ordering along the <111> direction, is the lowest energy of those considered. This ordered structure is shown in Figure 1. In addition, the band structure for this structure shows a pseudogap, seen in Figure 2, consistent with the observed transport behavior of Cr$_3$Al.

The SDW pseudogap also plays an important role in the semiconducting behavior, but this is difficult to measure experimentally. The Neel temperature of Cr$_3$Al is about 500°C, at which point the resistivity is already quite metallic [6]. For this reason, two previous studies on the resistivity around the Neel temperature came to different conclusions about the role of the SDW pseudogap on the semiconducting behavior [4,15]. Our theoretical results clearly suggest that antiferromagnetism is a necessary condition for the semiconducting behavior. Figure 3 compares the calculated density of states for antiferromagnetic and nonmagnetic Cr$_3$Al and shows that the pseudogap is eliminated in the nonmagnetic case.

In conclusion, we find that chemical ordering and antiferromagnetism work together to cause the unexpected semiconducting behavior in Cr$_3$Al.

References:

Thermoelectric Properties Measurement of 1D Nanostructures

CNF Project # 1854-09
Principal Investigator(s): Yaqiong Xu
User(s): Yunhao Cao, Yang Yang, Yaqiong Xu

Affiliation(s): Department of Electrical Engineering and Computer Science, Vanderbilt University
Primary Research Funding: Vanderbilt University
Contact: yaqiong.xu@vanderbilt.edu, yunhao.cao@vanderbilt.edu, yang.yang@vanderbilt.edu, yaqiong.xu@vanderbilt.edu
Web Site: http://eecs.vanderbilt.edu/people/yaqiongxu

Abstract:

One-dimensional (1D) nanostructures such as nanotubes, nanowires, and nanoribbons of different materials are intriguing significant attention because of their potential wide applications. One focus is their unique thermophysical properties, which are very different from those of their bulk counter parts [1]. Conventional techniques for thin film thermal properties measurements, like the \(3\sigma\) method, cannot be used readily for these 1D nanostructures due to the small sample size. We are developing a suspended microdevice for measuring thermal conductivity and Seebeck coefficient of various 1D nanostructures.

Research Summary:

Figure 1 shows the fabrication process of our suspended microdevice. We begin with the deposition of a 0.5 \(\mu m\) thick low stress SiNx film on both sides of a 100 mm diameter Si wafer using low pressure chemical vapor deposition (LPCVD) method. A 30 nm thick Pt film is then deposited on the SiN\(_x\) film by radio frequency (RF) sputtering. The Pt film is patterned by standard photolithography process and etched using ion milling. After stripping the photoresist, a 200 nm thick low temperature silicon dioxide (LTO) film is deposited on the patterned Pt layer by plasma enhanced chemical vapor deposition (PECVD). The LTO and low stress SiN\(_x\) films are then patterned by photolithography process and etched by reactive ion etching (RIE). After the photoresist is stripped, using the patterned SiNx as a mask, 10% tetramethylammonium hydroxide (TMAH) is used to etch the exposed Si region and the suspended structure is released when the Si substrate is etched away.

Figure 2 shows the scanning electron microscopy (SEM) image of boron carbide nanowire bridging two suspended membranes of our device. We use the same measurement method as described in Reference [2].

References:

High Resolution Reversible Color Images on Photonic Crystal Substrates

CNF Project # 1861-10
Principal Investigator(s): David Erickson
User(s): Pilgyu Kang

Affiliation(s): Sibley School of Mechanical and Aerospace Engineering, Cornell University
Primary Research Funding: This work was partially supported by the Air Force Office of Scientific Research through an STTR grant to Illuminaria LLC, under the Reconfigurable Materials for Cellular Electronic and Photonic Systems discovery challenge through and the US National Science Foundation through grant NSF-CBET-0846489 “CAREER: Optofluidics - Fusing Microfluidics and Photonics.”
Contact: de54@cornell.edu, pk344@cornell.edu

Abstract:
Here we demonstrate a technique for creating erasable, high-resolution, color images using transparent inks on self-assembled photonic crystal substrates. We exhibit a power-free fluidic infusion technique through the use of multi-oil inkjet printing for the creation of custom images with the resolution as high as 200 µm without the need for predefined template stamps. The substrates can be also returned to their initial state through the application of erasing oil. We expect that such a technique could find applications in the development of new flexible and stretchable drawing substrates and low power reflective display technologies.

Summary of Research:
A number of techniques for dynamically and spatially modulating the colors reflected off of photonic crystal-like substrates have been developed, for example, using electrical [1] and magnetic actuation [2] methods. The application of these external fields to drive the color change can be fast and provide good dynamic range but they require external power, an embedded method for spatially modulating the field, and are not directly applicable to writing substrates. Thus we exhibit a power-free fluidic infusion technique through the use of multi-oil inkjet printing for the creation of custom images with the resolution as high as 200 µm without the need for predefined template stamps [3]. The substrates can be also returned to their initial state through the application of erasing oil.

Figure 1 shows a sample polystyrene colloidal photonic crystal (CPC) substrate. The substrate fabrication technique exploits the capillary forces to drive the self-assembly [4] and we embed the final crystal structure in PDMS using a similar technique to that described by Fodouzi et al. [5]. From the Bragg equation locally swelling the lattice therefore will cause the reflected wavelength to increase. To accomplish this, we use a series of different silicone oils as “colorless inks” [3]. Figure 2 shows the reflectance spectrum obtained from an initially green CPC substrate for the range of commercially available silicon oils from the high molecular weight to the low molecular weight. The peak reflectance wavelength for all the oils used here is plotted in Figure 2 for both initially blue and green substrates.

Figure 1, top: Self-assembled colloidal photonic crystal substrates. Colloidal photonic crystal substrates were self-assembled on glass slides (5 x 5 cm) and are shown here in the initial amorphous state (left) and the crystallized state (right). After crystallization, the polystyrene spheres form a face-centered-cubic crystal structure which is fixed in a PDMS matrix. The substrate on the right exhibits a photonic bandgap at a wavelength of 489 nm.
To create high-resolution images on these substrates, we make use of a Dimatix Material Printer, which has the capability to deliver oils of different molecular weights and viscosities with high positional accuracy. Three different images of varying complexity and color range are recreated in Figure 3. The first image in Figure 3 shows the logos of Cornell University (which contains fine features and letters) transferred to the blue and green CPC substrate with a monochrome green and orange ink respectively.

The low vapor pressure of the low molecular weight oils can be exploited to erase transferred images and the reset the substrates without the degeneration of the original substrate or reduction in the quality of the reproduced images. As can be seen in Figure 4 the substrate is returned to the original color without a trace of the original image.

To conclude, in this work, we have demonstrated the use of self-assembled colloidal photonic crystal substrates to support high resolution, multi-color, stable but erasable images printed with transparent silicon oils of varying molecular weight. We expect that such a technique could find applications in the development of new flexible and stretchable drawing substrates and low power reflective display technologies.

References:


Fabrication of Superconducting Devices for Quantum Information Science

CNF Project # 1873-10
Principal Investigator(s): Britton L.T. Plourde
User(s): Joel Strand

Affiliation(s): Department of Physics, Syracuse University
Primary Research Funding: Intelligence Advanced Research Projects Activity (IARPA)
Contact: bplourde@phy.syr.edu, joel.strand@gmail.com
Web Site: http://www.phy.syr.edu/~bplourde

Abstract:

We are fabricating nanoscale superconductor tunnel junctions and microwave resonators for investigations in quantum information science. Such circuits have shown great promise in recent years for forming qubits, the elements of a quantum computer. We are developing architectures involving multiple superconducting qubits and microwave resonators. This involves a combination of photolithographic processing of large-scale features and electron-beam lithography for the tunnel junctions.

Summary of Research:

In recent years, circuits composed of nanoscale Josephson junctions have emerged as promising candidates for the element of a quantum computer, due to the low intrinsic dissipation from the superconducting electrodes and the possibility of scaling to many such qubits on a chip [1]. The quantum coherent properties the superconducting measured at temperatures below 50 mK with manipulation of the qubit state through microwave excitation.

We are working to develop architectures involving multiple superconducting qubits [2] coupled to multiple low-loss microwave resonators [3]. The coupling between each qubit and resonator leads to a vacuum Rabi splitting in the microwave transmission through the resonator when the qubit energy level difference is tuned to the characteristic frequency of the resonator. With the qubit detuned from the resonator, the qubit state can be probed by a dispersive shift of the resonator frequency [4].

We pattern these circuits at the CNF with nanoscale structures defined with electron-beam lithography integrated with photolithographically defined large-scale features. The junctions are fabricated using the standard double-angle shadow evaporation technique, in which a resist bilayer of copolymer and PMMA is used to produce a narrow PMMA airbridge suspended above the substrate. Evaporation of aluminum from two different angles with an oxidation step in between forms a small Al-AlOx-Al tunnel junction from the deposition shadow of the airbridge. We have developed a process for defining these junctions on the JEOL 9300 and we perform the aluminum evaporations in a dedicated chamber at Syracuse. We pattern large-scale features using the Autostep 200, with sputter deposition of Nb and NbN films in dedicated systems at Syracuse University. Measurements of these circuits are performed in cryogenic systems at Syracuse University, including a custom dilution refrigerator for achieving temperatures of 30 mK.

References:

Figure 1: Scanning electron micrograph of Al-AlO$_x$-Al Josephson junction.

Figure 2: Optical micrograph of superconducting qubit incorporating three Josephson junctions coupled to Nb microwave resonator.

Figure 3: Optical micrograph of superconducting qubit coupled through an interdigitated capacitor to Nb microwave resonator.

Figure 4: Measurement of vacuum Rabi splitting for superconducting qubit coupled to NbN microwave resonator.
Photonic Crystal Nanocavities for Solid State Quantum Optics

CNF Project # 1889-10
Principal Investigator(s): Antonio Badolato
User(s): Yiming Lai

Affiliation(s): Department of Physics and Astronomy, University of Rochester
Primary Research Funding: National Science Foundation
Contact: badolato@pas.rochester.edu, lmign@pas.rochester.edu
Contact: http://www.pas.rochester.edu/urpas/badolato_antonio

Abstract:
The radiative properties of an atom can be dramatically modified when it is coupled to an optical cavity [1]. Implementing such quantum optical effects in solid-state is essential for the realization of integrated quantum optical devices, including those relevant to quantum information science [2,3]. The success relies on the fabrication of state-of-the-art artificial atoms and nanocavities. Our artificial atoms are InAs/GaAs self-assembled quantum dots (QDs) grown by molecular beam epitaxy. Our nanocavities are formed by defects in two-dimensional photonic crystal slabs. Here we report on the fabrication of two types of photonic crystal nanocavities (PCNs) whose characteristics are crucial in solid-state quantum optics.

Summary of Research:
Optical cavities are characterized by two main quantities: the mode volume, that is, the spatial extent of the electromagnetic confinement, and the quality factor ($Q$), which is proportional to the photon cavity lifetime. When trapped for long time (high-$Q$) in small volumes, photons strongly interact with the host material and create significant nonlinear effects. PCNs with ultra-high-$Q$ and mode volume close to the diffraction limit ($\lambda/n^3$) have been achieved by several research groups [2,4]. High-$Q$s are made possible by suppression of the electric field Fourier components within the light zone. But this comes at a price: high-$Q$ PCNs are poorly coupled to the vertical direction (i.e. orthogonal to the slab). Here we report on the fabrication of L3 PCNs optimized for highest $Q$ (Figure 2a) and for highest far-field vertical collection (Figure 2b) [5].

The fabrication consists of the following steps: (i) We start with an epitaxially grown III-V semiconductor heterostructure that includes a layer of InAs/GaAs QDs in the middle of the slab (Figure 1a). (ii) After defining the PCN pattern on the resist (ZEP 520A) by electron beam lithography, (iii) we transfer the pattern into the semiconductor by chlorine-based inductively coupled plasma reactive ion etching (ICP-RIE). (iv) The Al$_x$Ga$_{1-x}$As ($x \approx 0.7$) sacrificial layer is removed by selective HF wet etching (Figure 1b).

![Figure 1: (a) Semiconductor heterostructure grown by MBE. (b) Cross section image of the PCN.](image1)

![Figure 2: SEM images of the L3 PCNs (a) optimized for highest $Q$ (b) optimized for far-field vertical collection.](image2)
Figure 2 shows the scanning electron microscope images of the fabricated PCNs. Figure 2(a) shows the high-$Q$ L3 PCN formed by three missing air holes in the hexagonal lattice of holes patterned in a $\lambda/n$ thick slab. The marked holes were shifted and shrunk to maximize the $Q$. Figure 2(b) shows the L3 PCN optimized for far-field vertical collection. Starting from the former design, Figure 2(a), the marked holes were enlarged. Figure 3 shows the normalized photoluminescence spectra of our PCNs. The carriers generated into the GaAs by a laser pump (650 nm) above the bandgap recombine into the QDs, which act as internal source for the PCN. Emission peaks are well fitted by Lorentzian curves. The typical $Q$s for high-$Q$ L3 PCN were resolution limited, $Q \approx 9000$ (solid line). As expected, a lower $Q \approx 5600$ (dashed line) was measured in L3 PCNs optimized for far-field, but a remarkable enhancement of light intensity was detected in the vertical direction.

We emphasize that light confinement in nanocavities relying only on index guiding is well understood, while current PCN understanding is much less mature because of the hybrid character of the confinement. (Photons are confined vertically by total internal reflection and laterally by Bragg reflection.) Our PCNs demonstrate that we can model and fabricate PCNs in GaAs heterostructures with specific functionalities. Such designs [2,5] are suitable for applications where light extraction is key such as single photon emitters [6].

References:

First-Principles Study of the Surface Chemistry of Metal-Oxide Nanostructures

CNF Project # 1998-11
Principal Investigator(s): Yongqiang Xue
User(s): Abraham Hmiel, Yongqiang Xue

Affiliation(s): College of Nanoscale Science and Engineering, State University of New York at Albany, Department of Nanoscience
Primary Research Funding: NYSERDA
Contact: xqxe@uamail.albany.edu, ahmiel@uamail.albany.edu, yxue@uamail.albany.edu
Web Site: http://www.albany.edu/~yx152122/

Abstract:

In this project, we utilize recent developments in density functional theory (DFT) and molecular dynamics (MD), including the self-consistent van der Waals (vdW) functional and the Effective Screening Medium (ESM) theory, to study the surface chemistry and wetting of H₂O on nanostructured TiO₂ surfaces and metal-decorated and biased TiO₂ surfaces. The energetics, kinetics and dynamics of the water monomer, dimer, small cluster, monolayer and multilayer on these nanostructured TiO₂ surfaces in the presence of surface defects and metal decoration will allow a more complete understanding of the key surface processes that will govern the utility of these devices.

Summary of Research:

The rutile TiO₂ <110> surface, apart from being a prototypical model for study in metal-oxide interfaces, is technologically relevant in energy applications like fuel cells and photocatalytic water splitting [1]. Current carbonless support materials in development for fuel cell applications make use of TiO₂ nanorods > 10 nm in diameter which can be modeled as surface slabs in DFT. The current state of knowledge about this surface’s electronic structure is significant, but falls short in some areas, namely, the chemical reactions that take place at a water interface in the presence of surface defects or adsorbed metals and at electrical bias. Developments in density functional theory (DFT) allow for an accurate self-consistent treatment of van der Waals (vdW) dispersion effects between water molecules and other bound systems whose character is neither covalent, ionic, nor metallic [2]. Furthermore, the ability to simulate DFT with a screened electric field is useful for the accurate treatment of real devices, and a modification to the electrostatic boundary conditions to achieve this end has been grafted onto mainstream DFT code packages [3].

We use the SIESTA[4] code on the CNF cluster with Perdew-Burke-Ernzerhof (PBE) and vdW [2] exchange-correlation (XC) functionals to relax rutile and anatase surface slabs of varying thickness and test for convergence, with primary focus on the rutile <110> surface slab. We use Troullier-Martins-style nonlocal norm-conserving pseudopotentials to screen the ionic nuclei with core electrons.

We used 3, 4, 5, 6, and 7 surface trilayers for this study, which determined that the surface energy oscillates around an asymptotic value of about 0.42 eV/surface unit cell for PBE-DFT, in agreement with [5]. The bottom trilayer of the surface slab was held fixed to the bulk positions for each particular exchange-correlation functional examined. Odd and even numbers of trilayers have different overall effect
on the electronic structure and relaxed geometries of the surface slab. This result was reinforced by our calculation of small-diameter rutile TiO$_2$ [001] nanowires with $<$110$>$ facets of varying size which concluded that odd or even numbers of surface titanium sites on each facet had two pronounced effects on the electronic structure. The bandgap for even TiO$_2$ NWs was indirect and that of the odd faceted nanowires was direct as illustrated in Figures 2 and 3.

An in-depth study of the electronic structures and geometry effects present in TiO$_2$ NWs of different surface terminations and diameters is currently in progress. Our future publication will draw attention to the distribution of bond lengths in each nanowire, the projected density of states (PDOS) of the Ti 3d and O 2s orbitals by location on the nanowire, and the local density of states (LDOS) at the conduction and valence bands in comparison with the rutile $<$110$>$ surface. It will be part of our future work to study how the inclusion of the vdW functional affects the geometry and electronic structures of metal oxides and then proceed into computing their wetting properties.

We tracked the changes to the geometries and energetics of water dimers with different XC-functionals, and basis sets, including several different parameterizations of the vdW functionals that are supported by SIESTA. The reproduced bond angles, dipole moments, geometries, and energetics of the water dimer system compare quite well to experiment and to theory in the complete basis set limit. The results show that the O-H binding energies are improved for the functional with vdW correlation, and little is gained in varying the exchange part. The bond angles, dihedral angle of the dimer arrangement, and bond lengths are also slightly improved over GGA-DFT. Benchmarks indicate that the inclusion of vdW correlation versus GGA-style correlation represents an order of 10 times more computational effort required to set up the exchange-correlation term in the Hamiltonian. Because the exchange-correlation terms are dependent on the size of the real-space grid in SIESTA, the increase in computation time of a surface slab or molecule will be different depending on the size of the simulation cell. SIESTA’s CPU scaling shows good performance for up to 16 nodes in parallel, and 4 or 8 CPUs per task seems to have an optimal time elapsed per total computational effort ratio when parallelized over k-points.

References: