Session I – Devices @ MRGN 129, Purdue University

1.1 Proposal for an All-Spin Transistor with Built-In Memory

Author: Behtash Behin-Aein

Time: 9:30am – 9:45am

Abstract:

The possible role of spin as an alternative to charge for logic applications is well recognized. However, spin-based proposals typically use spin only as an internal variable, the terminal quantities for each individual logic gate still being charge-based. The purpose of this paper is to present a concept for implementing an All-Spin Transistor (AST) where information stored in an input magnet is used to generate a spin current that can be routed along a spin-coherent channel to any desired location where it determines the final state of the output magnet. The magnets act like digital spin capacitors analogous to the charge capacitors in conventional digital circuits, while the spin currents play the role of charge currents. Although the proposed device operation has not yet been demonstrated experimentally we argue that it should be feasible using simulations with an experimentally benchmarked model based on the established physics of spin-torque switching. We further argue that this device if implemented, should exhibit the five essential characteristics for logic applications, namely non-linearity, gain, concatenability, feedback elimination and a complete set of Boolean operations. The proposed scheme should afford a versatility comparable to standard charge-based architecture while having the potential for low power operation and continued scaling.

1.2 Simulation study and tool development for ultra-scaled In-As HEMTs

Author: Neerav Kharche, Mathieu Luisier, and Gerhard Klimeck

Time: 9:45am – 10:00am

Abstract:

III-V High Electron Mobility Transistors (HEMTs) have recently emerged as potential candidates for high-speed, low-power logic applications beyond Si-CMOS technology. The standard techniques such as drift-diffusion cannot capture quantization of the energy levels resulting from the strong confinement of the electrons in a quantum well channel and tunneling currents in these nanoscale devices. Thus the need to develop modeling techniques to aid experiments and explore novel device designs arises. Here we employ a real-space effective mass 2-D Schrödinger-Poisson solver to analyze transport characteristics of InAs HEMTs. For computational reasons the simulation domain is restricted to the gate contact region and source/drain contacts are modeled via two series resistances. The simulation approach is verified for recently reported InAs HEMTs where a good quantitative match to experimental data is obtained. The device simulator can be used to gain deeper insight into the electron transport and thereby to design the device for optimal performance when scaled below 20nm regime. A web-based interactive version of the tool will be available shortly on the website www.nanohub.org.

1.3 Analysis and characterization of graphene-on-substrate devices

Author: Dionisis Berdebes and Mark Lundstrom

Time: 10:00am – 10:15am

Abstract:

Transport phenomena in graphene monolayers have received a lot of attention due to the extremely high mobility, the simple planar geometry and the intuitive physical behavior of this material system. Of special interest is the understanding of the temperature-dependent scattering mechanisms that degrade the current transport. This work is focusing on the understanding of these mechanisms, by combining experimental input over a range of devices of different dimensions with the Landauer theory for conductance, away from the Dirac minimum. The main physical parameter that we employ for the characterization of the transport properties is the mean free path. We investigate 4 different devices by extracting the mean free path as a function of energy and by exploring the monotonicity of the temperature dependence of conductance. A single scattering scheme cannot explain our input. The characterization of the devices with the use of the mean free path instead of mobility as the principal physical quantity is, justifiably, a more promising approach. Samples with a very weak dependence of the mean free path on energy, suggest that further discussion is needed.

1.4 Importance of Diameter Distributions for Directly-Bridging CNT Array transistors

Author: Shuaib Salamat

Time: 10:15am – 10:30am

Abstract:

The fundamental notion that Single-Wall Carbon Nanotubes (SWNT) behave as Schottky Barriers (SB) devices led to use of average diameter of array of CNFET as representative of the device. The diameter of CNT, however, besides the nature of source/drain metal determines the height of SB at metal nanotube interface. We use perfectly aligned parallel array of SWNTs as the channel. The diameters in these CVD grown SWNTs, are widely distributed. For CNFETs transistors, using similar device geometries and contact material, we observe variation in Threshold Voltage (VT), On-current (Ion) and device resistance (Rd). Average Diameter of the CNTs, making up these transistors, is about the same, and therefore could not account for variations in the device characteristics. Using measured diameter distributions for various devices we carry out systematic simulations to determine devices' characteristics and ascertain the variations in Ion, VT and Rd that result from variation in diameter distribution of the starting device.

1.5 Evanescent-mode Cavity Based Tunable RF MEMS Resonators and Filters

Author: Xiaoguang (Leo) Liu

Time: 10:45am – 11:00am

Abstract:

In this paper we present the modeling, design, fabrication and measurement of continuously tunable evanescentmode cavity-based tunable resonators and filters with integrated RF MEMS tuners and with very high quality factors (Q). Tunable resonators with 2.8 : 1 (5.0-1.9 GHz) tuning ratio, Q of 300- 650 and 1.8 : 1 (6.2-3.4 GHz) tuning ratio, Q of 460-530 are demonstrated. The required bias voltage is less than 120 V. A continuously tunable 2-pole filter from 3.76 GHz to 5.17 GHz with bandwidth of 0.7%and insertion loss less of than 4 dB is also demonstrated. Mechanical stability measurements show that the tunable resonators/filters exhibit very low frequency drift. This is partly due to the employed single-crystal silicon actuators coated with thin gold films. Such tunable resonators and filters will be an essential part of next generation reconfigurable radio front-ends.

1.6 Simulation study of Schottky barrier III-V MOSFETs

Author: Himadri Pal

Time: 11:00am – 11:15am

Abstract:

Quantum transport in InGaAs channel metal source/drain Schottky barrier MOSFET is simulated using the NEGF formalism in a double-gate device framework. The subthreshold and gate overdrive characteristics are compared to doped source/drain InGaAs MOSFETs. The Schottky FETs show enhanced peak transconductance and higher on currents for Schottky barrier energy below 0.1eV. InGaAs channel Schottky FETs also has better subthreshold characteristics than their Si channel counterparts. A study of channel thickness scaling suggests bandstructure non-parabolicity affecting InGaAs Schottky FET performance at extremely thin body devices.

1.7 Design of multimode three-dimensional photonic crystal cavities for enhanced anti-Stokes Raman scattering

Author: Jing Ouyang

Time: 11:15am – 11:30am

Abstract:

Multimode hollow cavities in three-dimensional (3D) photonic crystals (PhCs) are designed for achieving enhanced anti-Stokes Raman scattering, which requires a cavity to have three modes with equally spaced resonant frequencies. Cavities in 3D PhCs can be free from radiation losses associated with the ones in 2D slab PhCs, thus allowing more flexibility in design and tuning. We first tune all the mode freuqencies simultaneously by changing the material and geometry of the cavity based on perturbation theory. Spectral spacings between the multiple modes are adjusted according to the symmetry, volume and field distribution of their mode profiles. Spatial overlaps of the three active cavity modes are calculated as a measure of how well the anti-Stokes generation is. The frequency and field distribution of the resonant modes are computed by solving Maxwell's equations in the frequency domain.

1.8 Online Modeling and Simulation Tool for a MEMS Thermal Actuator by Integrating Distributed and Lumped Analyses

Author: Fengyuan (Thomas) Li and Jason V. Clark

Time: 11:30am – 11:45am

Abstract:

We are developing an online tool which allows both novices and experts to quickly and fairly accurately model and simulate an electro-thermo-mechanical microdevice by integrating distributed and lumped analyses. Our hybrid tool couples distributed and lumped analyses. Using distributed analysis, we model the temperature distribution caused by electric current passing through a flexure beam. Then using lumped analysis, we model the thermal expansion that was caused by the temperature distribution. This fundamental electro-thermal beam element is found in many MEMS. To validate our hybrid method, we

use the method to model an electro-thermal actuator that has been reported to characterize nanowires and nanotubes. We verify our tool against the experimental results and against full distributed analysis that we have performed using COMSOL .

Typical thermal actuators provide O(10^{-4}) Newtons of force, which is about three orders of magnitude larger than the popular electrostatic comb drive actuator. Distributed analysis (or finite element analysis) is commonly used to model electro-thermal-mechanical actuators. It provides detailed results, such as the electric and potential field calculations, the mechanical stress and strain distribution calculations, the charge distribution calculations, etc., but it requires a large amount of computational memory and time. The lumped analysis has also been used to model the same electro-thermal actuator. The relative error of the tip stroke between their lumped analysis to full distributed analysis is 2.9%. We plan to implement their method online as a second modeling option.

For faster results over full analysis, we only use distributed analysis where necessary. Another benefit is a lower computer memory requirement. Our tool is about 10 times faster than pure distributed analysis. The accuracy of our integrated distributed-lumped tool is within 6% of full distributed analysis and within 12% of experiment for the normal operating temperature (less than 1100 degree Celsius). We believe that most of the 12% error is due to geometric and material property mismatches between the true actuator and its simulated counterpart. Such mismatch is due to process variations. The 6% error to full distributed analysis is mainly due to the ideal assumptions made in lumped analysis, such as the linear beam model. By using linear beam model in full distributed analysis, the relative error drops to 0.97%. Beyond the normal operating temperature (more than 1100 degree Celsius), the experimental results of the tip stroke are more than 30% smaller than the simulation results in either our integrated distributed-lumped method or the full distributed method with nonlinear beam model. The possible reason of self-annealing and localized melting at the grain boundaries caused by second breakdown in poly-silicon under high temperature (about 1300 degree Celsius) is discussed. Our tool will soon be available on the nanoHUB.

1.9 A tool for 1D heterostructures: 1DHetero

Author: Jean Michel Sellier

Time: 11:45am – noon

Abstract:

Experimental technologies such as molecular beam epitaxy enable the deposition of compound semiconductor materials with atomic precision. Heterostructures result from the deposition of dissimilar materials and are of great importance from both scientific and industrial points of view.

A tool has been implemented to simulate such heterostructures and is deployed on nanoHUB website: 1DHetero.

In this talk the author is going to show how such a simulator looks like and how to use it for concrete simulations. The author will focus on the use of the GUI and will show some results to prove the reliability of the tool.

Lunch and Poster Exhibit @ MRGN Lobby, Purdue University

Time: noon – 1:30pm

Presentation Session II – Properties of Materials for Devices @ MRGN 129, Purdue University

2.1 Thermal conduction in metallic nanostructures via molecular dynamics

Author: Ya Zhou, Benjamin Anglin, and Alejandro Strachan

Time: 1:30pm – 1:45pm

Abstract:

We use nonequilibrium molecular dynamics (MD) to characterize phonon thermal conduction of Al nanostructures and the role of interfaces in metallic nanolaminates. We characterize size and temperature dependence of phonon thermal properties of pure Al samples, and thermal conductivity of Al/Al* (where Al* differs from Al only in its mass) and Al/Ni nanolaminates. The interfacial resistivity depends on the direction of the heat flux; this is the first molecular level characterization of such thermal diode behavior in a realistic three dimensional material. Simple, additive models are proposed which provide good estimates of the thermal conductivities of the nanocomposites in terms of the behaviors of the constituent components and interfaces. The thermal role of electrons is taken into account using a recently proposed mesodynamics method called dynamics with implicit degree of freedom (DID).

2.2 Multi-probe Interface Characterization of $In_{0.65}Ga_{0.35}As/Al_2O_3$ MOSFET

Author: Dhanoop Varghese

Time: 1:45pm – 2:00pm

Abstract:

Through a combination of measurement techniques, we study the interface properties of $In_{0.65}$ $Ga_{0.35}As$ transistor with ALD deposited Al_2O_3 gate dielectric. We show that the interface trap density at $In_{0.65}$ $Ga_{0.35}As/Al_2O_3$ interface can be relatively high, but the transistor still exhibits inversion characteristics. A detailed profiling of the interface traps show that majority of the interface traps are donor-like, and explains the absence of Fermi level pinning in spite of the high interface trap density.

2.3 A bottom-up approach to thermoelectricity and its application to molecular thermoelectric devices

Author: Lutfe Siddiqui, Abu Naser M. Zainuddin, and Supriyo Datta

Time: 2:00pm – 2:15pm

Abstract:

Thermoelectric devices can play an important role in meeting the energy challenges of the future. It has been identified that the figure of merit ZT of such class of devices needs to exceed 3 for them to become a viable technology. In pursuit of achieving this end, thermoelectric phenomena in different structures ranging from thin-film devices to quantum-dot superlattices, and also, across different dimensions and length-scales ranging from bulk devices to molecular conductors are being investigated. To evaluate the merit of these different ideas, and also, to compare them against each other seamlessly, the bottom-up approach to electronic transport can play a crucial role by virtue of a unified point of view that it lends in understanding electronic transport across different structures, dimensions, and length-scales. In this presentation, we will illustrate this approach and apply it to explore the prospect of molecular thermoelectric devices.

2.4 Characterization of amorphous silica using molecular dynamics

Author: Ravi Pramod Vedula, Nathan Anderson and Alejandro Strachan

Time: 2:15pm – 2:30pm

Abstract:

We use molecular dynamics with the reactive force field ReaxFF to predict the structure of amorphous silica and formation energy for point defects. The local structure of amorphous silica determined using Reactive Force Field molecular dynamics simulations was compared to neutron diffraction and NMR spectroscopy observations. Amorphous silica was generated by heating alpha quartz to 4000K and then cooling it to 300K using NPT runs at the rate of 50k/20ps. The structural properties of amorphous silica obtained were in good agreement with the experimental results. The radial distribution function of our structures had peaks in excellent agreement with that obtained experimentally. The mean Si-O-Si bond

angle was found to be 149.58 as compared 148 obtained experimentally. The effect of simulation cell size on the local structure was also investigated. The vacancy formation energy for O and Si vacancy has been calculated.

2.5 Phase Field Micro-Mechanical Model (PFMM): Performance Analysis and Interface Effects in the Plastic Response of FCC Crystalline Materials

Author: Abigail Hunter

Time: 2:45pm – 3:00pm

Abstract:

The inelastic response of crystalline materials is mediated by dislocation motion and their interaction with defects, such as second phase particles, dislocations, grain boundaries and voids. This is particularly important when the scale of the volume of analysis approaches the microstructure scale as in micron and sub-micron size devices, such as micro-electrical-mechanical systems (MEMS), and in nanocrystalline materials.

3D phase field micro-mechanical simulations of the mechanical response of passivated thin films at micron and sub-micron scales will be presented. The simulations show the effects of interfaces and volume confinement on dislocation structure, evolution and mobility that result in size dependent behavior over length scales ranging from nanometers to micrometers.

Additionally, a performance analysis of the 3D phase field model will be presented. Performance on multiple architectures, including GigE, Infiniband, and SiCortex interconnects available on Purdue computing clusters, will be discussed. Data will show how the run times and scalability of the model varies over the different interconnects for several simulation sizes.

2.6 Application of Tight-Binding based VCA model to Si-Ge systems

Author: Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier and Gerhard Klimeck

Time: 3:00pm – 3:15pm

Abstract:

Shrinking device dimensions is making it necessary to look for alternative approaches to increase Ion and mobility of Silicon FETs. SiGe/Si core/shell nanowire FETs are proving important since they have higher Ion and mobility compared to silicon and at the same time with a small silicon capping layer it is easy to grow an oxide layer. This work focuses on the application of Tight-Binding (TB) based Virtual Crystal Approximation (VCA) to understand the electronic structure of SiGe systems and to use the developed model to understand quantum transport in SiGe nanowire FETs. The bulk theoretical results

have been benchmarked against the experimental results. Once we are confident about the electronic structure model we used the Top-of-the-Barrier ballistic quantum transport model, to study the improvement in SiGe n-type nanowire FETs compared to similar n-type silicon FETs.

2.7 Strain relaxation in Si/Ge/Si nanoscale bars from molecular dynamics simulations

Author: Yumi Park and Alejandro Strachan

Time: 3:15pm – 3:30pm

Abstract:

We use molecular dynamics (MD) with the reactive interatomic potential ReaxFF to characterize the local strains of epitaxial Si/Ge/Si nanoscale bars as a function of their width and height. While the longitudinal strain (along the bars length) is independent of geometry, surface relaxation leads to transverse strain relaxation in the Ge section. This strain relaxation increases with increasing height of the Ge section and reduction of its width and is complete (i.e. zero transverse strain) for roughly square cross-sections of Ge leading to a uniaxial strain state. Such strain state is desirable in some microelectronics applications. From the MD results, which are in excellent agreement with experiments, we derive a simple model to predict lateral strain as a function of geometry for this class of nanobars.

2.8 Orthogonal tight binding for bandstructure of strained Si/ strained Ge/ strained Si hetero nanowires

Author: Amrit Palaria

Time: 3:30pm – 3:45pm

Abstract:

One of the most promising extensions to conventional CMOS technology being currently investigated is the 1-D nanostructure FET. One design that can combine confinement properties of 1-D nanostructures and strain properties of heterostructures is the strained Si/ strained Ge/ strained Ge hetero-structure nanobar FET. In this presentation, I discuss the challenges of simulating the bandstructure and electrical transport properties of a realistic s Si/ s Ge/ s Si heterostructure nanowire within the bottom up paradigm using orthogonal tight binding. It is found that the basic concept of orthogonal tight binding needs rethinking mainly due to presence of surface bonds. I propose the adaptive tight binding for simulating bandstructure of materials with non-bulk bond environments.