Electronic Materials and Photonics Division
Room: 14 - Session EM-WeM

Charge Transport in Disordered Materials

Moderator: Michelle Paquette, University of Missouri-Kansas City

8:00am **EM-WeM1 Electrons and Phonons in Amorphous Semiconductors**, ***David Drabold***, *K. Prasai*, Ohio University, *P. Biswas*, University of Southern MIssissippi **INVITED**

The coupling between lattice vibrations and electrons is one of the central concepts of condensed matter physics. The subject has been deeply studied for crystalline materials, but far less so for amorphous and glassy materials, which are among the most important for applications. In this talk, we explore the electron-lattice coupling using current tools of first-principles computer simulation. We choose three materials to illustrate the phenomena: amorphous silicon, amorphous selenium, and amorphous gallium nitride. In each case, we show that there is a strong correlation between the localization of electron states and the magnitude of thermally-induced fluctuations in energy eigenvalues obtained from density-functional theory (i.e. Kohn-Sham eigenvalues). We provide a heuristic theory to explain these observations. The case of amorphous GaN, a topologically disordered partly ionic insulator, is distinctive compared to the covalent amorphous systems. We close by showing how the optical gap of an amorphous semiconductor can be computationally engineered with the judicious use of Hellmann-Feynman forces (associated with a few defect states) using molecular dynamics simulations. These forces can be used to close or open an optical gap, and identify a structure with a prescribed gap. We use the approach with plane-wave density functional methods to identify the conducting state of a conducting bridge memory material: Ag-doped $GeSe_3$.

K. Prasai, P. Biswas and D. A. Drabold, *Electrons and Phonons in Amorphous Semiconductors*, Semicon. Sci. Tech. **31** 073002 (2016).

8:40am **EM-WeM3 Percolation Resistivity in Nanostructured Transparent Conductor Networks Consisting of Curvy Nanowires**, ***Junying Li***, *C. Ying, J. Hicks, A. Ural*, University of Florida

Transparent, conductive electrodes have many applications in electronic and photonic devices such as touch screens, solar cells, LEDs, and photodetectors. Metal nanowire networks are promising candidates for these applications as a replacement for indium tin oxide, which has problems such as high cost, scarcity, and brittleness. The conduction in metal nanowire networks is governed by percolation theory.

In most computational work, nanowires in these networks have been modeled as straight "sticks". However, in real experiments, individual nanowires are not perfectly straight, but exhibit some degree of curviness. In this work, we perform systematic Monte Carlo simulations to study the effect of nanowire curviness on the scaling of percolation resistivity in nanowire networks. We generate the curved nanowires using 3rd-order Bézier curves. These curves are endowed with a curviness angle property that specifies how far away the two intermediate control points of the Bézier curve may lie, in the tangential sense, from a straight path connecting the two ends of the curve. The curviness angle is varied to obtain networks of differing values of curl ratio, which is defined as the ratio between the curved length of a nanowire and the straight distance between its two ends.

We find that, for random networks, the resistivity of the network increases with increasing nanowire curviness and the resistivity exhibits an inverse power law dependence on the curl ratio. We also find that the value of the extracted inverse power law critical exponent is not universal, but depends on other nanowire and device parameters. As a result, we also study the effect of nanowire density, nanowire length, device length, device width, and nanowire alignment angle on the scaling of network resistivity with nanowire curl ratio.

Curviness results in two competing effects on the percolation resistivity. First, curviness decreases the effective length of the nanowire between its two ends, which increases the resistivity. Second, it increases the effective width of the nanowire, which decreases the resistivity. For networks with aligned nanowires, we find that increasing the curviness decreases the resistivity, indicating that the second effect starts to dominate. By simulating networks with varying values of alignment angles, we study the crossover from the first to the second regime.

These results show how the degree of curviness of individual nanowires contributes to the macroscopic resistivity of the network. They also show that computational studies are an essential tool for providing insight into the percolation transport in transparent, conductive nanowire networks.

9:00am **EM-WeM4 Surface Chemical Control of Charge Transport and Infrared Plasmonic Response in Nanocrystal Thin Films**, ***Dmitriy Boyuk***, *W. Hu, M.A. Filler*, Georgia Institute of Technology

Infrared plasmonic nanocrystal thin films are promising materials for harvesting thermal radiation, but their use requires an ability to simultaneously control nanocrystal carrier density and interfacial charge transport. Here, we combine *in situ* infrared spectroscopy and nanoscale four-point probe measurements to show the intimate interplay between nanocrystal surface chemistry, the localized surface plasmon resonance (LSPR), and thin film resistivity. Indium tin oxide (ITO) nanocrystals synthesized via colloidal methods exhibit LSPRs tunable in the mid-infrared (from 0.2 to 0.6 eV) and serve as model infrared plasmonic materials with which to study these effects. Removal of surface hydroxyl groups, via reaction with metal alkyl species (e.g., trimethylaluminum), and formation of a monolayer of oxygen-metal surface bonds (e.g., Al-O) reduces the number of nanocrystal surface traps. The corresponding increase in carrier density is evidenced by a clear blue shift and increase in intensity of the LSPR. This monolayer surface treatment decreases nanocrystal film resistivity by two orders of magnitude (to 1×10^{-2} ohm-cm). We further demonstrate that conformal coatings (e.g., of Al_2O_3 or ZnO) permit control of nanocrystal thin film resistivity without modifying LSPR energy, a capability that allows us to independently engineer light absorption and device properties. We also find that these plasmonic nanocrystal films exhibit a photoconductivity in response to mid-infrared light illumination.

9:20am **EM-WeM5 Study of Cation Exchange and Transport in Crystalline Solids Through Density Functional Theory Calculations**, ***Daniel Dumett Torres***, University of Illinois at Urbana-Champaign

Ion transport is closely tied to chemical transformations of crystalline ionic solids such as impurity doping and ion exchange. In order to introduce heteroatoms and other impurities into a crystal it is necessary to displace ions, create vacancies, and fill vacancies many times to achieve a significant degree of transformation. Thus ionic mobility plays a deterministic role both as to how fast a transformation occurs and the achievable extent of doping/exchange in a given system. For example exchange of Cd^{2+} for Cu^{+} in CdSe nanocrystals occurs rapidly and full conversion is ultimately reached. However replacing Cd^{2+} for Hg^{2+} does not reach completion and proceeds more slowly. A full explanation for how these two processes differ must address the mobility difference between Hg^{2+} and Cu^{+} through the Se^{2-} sublattice.

As a separate example: fast ion conduction relies on there being extensive ion transport in a solid. Such transport could be facilitated by cooperative effects, low ($<k_bT$) activation energy barriers against ion migration, or a combination of these and other factors. An understanding for how ionic mobilities differ and how they might be manipulated or enhanced will guide the design of materials such as nanoscale semiconductors for applications in optoelectronics, solid state battery electrolytes, and thermoelectrics. Specifically, control over superionic phase transitions can make new materials available for applications in solid state electrolytes by permitting new superionic conductors to be realized at working conditions as opposed to at elevated temperatures.

The approach is to employ density functional theory (DFT) electronic structure calculations for the elucidation of ion conduction trends in $Li_xCu_{2-x}Se$. The $Li_xCu_{2-x}Se$ alloys vary in their fraction of Li^{+} or Cu^{+} cations both of which are mobile and thus apt for a study into tuning ion mobility. Total energies from DFT calculations for a large set of $Li_xCu_{2-x}Se$ structures permit the identification of factors that promote or inhibit ion mobility. By varying both the cation locations and cell parameters the energetic penalties associated with pushing cations from their relaxed positions into interstitial sites can be obtained. Coupled with a exploration of the $Li_xCu_{2-x}Se$ compositional range, the DFT energies reveal the best alloys for cation transport that have the lowest energetic penalties and smallest activation barriers. Complementary calculations in which the simulation cell volume is increased or decreased study the effects of tensile and compressive strain respectively; the calculated energies inform how strain and pressure can be used to control ion conduction.

9:40am **EM-WeM6 Probing Charge Transport in Amorphous Hydrogenated Boron Carbide**, ***Gyanendra Bhattarai***, *S. Dhungana, R. Thapa, T.D. Nguyen, A.N. Caruso, M.M. Paquette*, University of Missouri-Kansas City

Amorphous hydrogenated boron carbide is a complex disordered semi-insulating material being studied for neutron detection applications owing to its high thermal neutron absorption cross-section and high resistivity. Optimizing its charge transport properties, including charge carrier mobility, lifetime, and mobility-lifetime product, will be essential to successful

detector implementation. Tuning these properties requires a clear understanding of the disorder in this solid, as well as charge injection and hopping via localized states, and how these phenomena lead to difficulties in experimental design as well as analysis of charge transport measurements. This contribution will present an overview of the challenges and nontrivialities in establishing electrical contacts and determining charge transport properties introduced by the disorder in the material, and our approaches to measurement and analysis.

11:00am **EM-WeM10 On the Abnormality in Mobility of ZnO Thin Film Transistors Based on Sol-Gel Deposited Channel Layers**, ***Vahid Mirkhani***, *K. Yapabandara, S. Wang, M.P. Khanal, S. Uprety,* Auburn University, *M.H. Sk,* Qatar University, Qatar, *A. Ahyi, M.C. Hamilton, M. Park,* Auburn University

Extensive research has been conducted on zinc oxide (ZnO) thin film transistors (TFTs) for the last couple of decades. Solution processes such as sol-gel are popular fabrication methods among researchers due to their simplicity and economical aspects. We have observed an abnormality in transconductance and mobility curve of the TFT with a channel layer prepared through sol gel spin coating process. Transconductance and mobility curves, determined from transfer characteristics, exhibit two peaks, instead of an expected single peak. We have rationalized the phenomenon by pondering the ZnO-ZnO interfaces. During the ZnO thin film deposition process, the spin coating and calcination steps are repeated multiple times in order to achieve a desirable layer thickness. When a layer is deposited, prior to the second spin coating step, the vacancies on the layer surface (comprised of grain boundaries of different grains) act as active sites, adsorbing molecules from the ambient. The adsorption of gasses such as oxygen and water molecules on ZnO structure surfaces has been studied for several decades; although the detailed kinetics and chemical reactions are debatable. Moisture and oxygen may be chemisorbed on the surface by receiving an electron and form a trapped negative ion on the surface, forming a depletion region at the surface of the layer. Oxygen may capture an electron and react with oxygen vacancies (V_O and V_O^+), in order to form chemisorbed ions such as O^-, O^{2-} or O_2^-, whereas H_2O may form OH^- on the surface. Potential barriers created at the interlayer interfaces are wider and higher than the regular barriers created at the grain boundaries in the bulk. The interlayer interface depletion layers formed by negative ions will not be affected by the annealing process due to their stability at room temperature. Thus, the initial ZnO-ambient interface (prior to the next layer-deposition process) evolves into the ZnO-ZnO interlayer interface. The significance of the depletion layers at the ZnO-ZnO interfaces becomes evident when the carriers are not able to drift across these interfaces at gate voltages smaller than a critical voltage (V_C). As the gate voltage increases, the width of the depletion regions decrease and carriers are able to tunnel through the barriers with ease and utilize all the deposited layers as a single channel and hence, an increase in the transconductance and mobility and later, a second peak. It is proposed that the first peak is related to the formation of the channel in the top layer and the second peak is assigned to all the deposited layers acting as a single-layer-channel.

11:20am **EM-WeM11 Electrical Characterization and Localized Density of States Extraction of Thin-Film Transistors Based on Sol-Gel Derived ZnO Channel Layers with Different Annealing Temperatures**, ***Shiqiang Wang****, R. Cheng, M.C. Hamilton, V. Mirkhani, K. Yapabandara, S. Uprety, A. Ahyi, M. Park,* Auburn University, *M.H. Sk,* Qatar University, Qatar

We report on the fabrication and electrical characterization of bottom gate thin-film transistors (TFTs) based on sol-gel derived ZnO channel layer. The effect of annealing of ZnO active channel layers on electrical characteristics of the ZnO TFTs was systematically investigated. Photoluminescence (PL) spectra indicate that the crystal quality of the ZnO improves with increasing annealing temperature. Both the device turn-on voltage (V_{on}) and threshold voltage (V_T) shift to a positive voltage with increasing annealing temperature. As annealing temperature is increased, both the subthreshold slope (*SS*) and the interfacial defect density (D_{it}) decrease. The field effect mobility (μ_{FET}) increases with annealing temperature, peaking at 800 ℃ and decreases upon further temperature increase. Besides that, the temperature dependent field effect measurement (from 296 K to 330 K) was used to gain an insight on the annealing temperature effect on sol-gel derived ZnO TFTs electrical characteristics. The conduction processes in these TFTs are thermally activated and the drain current, especially in subthreshold regime, obeys Arrhenius equation. Thermal activation energy and a corresponding prefactor parameter were extracted from temperature dependent field effect measurement. The Meyer-Neldel (MN) rule widely observed in the intrinsic material property study is also obeyed by the relation between thermal activation energy and the prefactor parameter. By combing the MN rule and applying the self-consistent procedure, the localized sub-gap density of states (DOSs) of different temperature annealed sol-gel derived ZnO TFTs were successfully extracted. The DOSs for subthreshold regime decrease from 10^{19} $eV^{-1}cm^{-3}$ level to 10^{17} $eV^{-1}cm^{-3}$ level with increasing annealing temperature from 600 ℃ to 800 ℃ and no substantial change was observed with further temperature increase to 900 ℃. The results show that DOSs decrease with annealing temperature increase in general, but annealing at a very high temperature may not be beneficial to reducing DOSs. It was found that the TFTs with ZnO layers annealed at 800 ℃ for one hour shows the best electrical performance with the highest field effect mobility and lowest localized DOSs.

11:40am **EM-WeM12 Real-space Characterizations of Photo-generated Carriers in P3HT-based Nanostructures using Kelvin Probe Force Microscopy**, ***Eunah Kim****, S. Kwon, D.H. Kim,* Ewha Womans University, Republic of Korea, *H.-H. Park,* Korea Advanced Nano Fab Center, Republic of Korea, *J. Kim,* Incheon National University, Republic of Korea, *D.-W. Kim,* Ewha Womans University, Republic of Korea

Organic-inorganic hybrid nanostructures have been proposed to improve the performance of organic photovoltaic devices. In this work, we investigated creation and transport behaviors of photo-generated carriers in P3HT-based hybrid nanostructures, such as P3HT-coated Si-nanopillar (NP) arrays and P3HT layers with embedded upconversion nanorods (UCNs). Optical resonance strongly concentrated incident light in the Si NPs, significantly increasing the number of photo-carriers near the NPs. The UCNs converted near-infrared (NIR) light to visible light . We studied spatial distribution of the surface photovoltage (SPV) in the P3HT/Si-NP and P3HT/UCN samples using Kevin probe force microscopy. The magnitude and sign of SPV are determined by the number of the photo-carriers and band profiles near the sample surface [1-3]. Large SPV values appeared in the P3HT layers near the Si NPs under illumination of visible light and near the UCNs under illumination of NIR light in the P3HT/Si-NP and P3HT/UCN samples, respectively [3,4]. This suggested that the concentrated light in the NPs and photon upconversion in the UCNs increased the local density of photo-carriers. Our work shows that the scanning probe microscopy technique can visualize the creation and transport behaviors of photo-generated carriers in nanostructures.

1. E. Kim et al., *Curr. Appl. Phys.***16**, 141 (2016).

2. M. Gwon et al., *Sci. Rep.***5**, 16727 (2015).

3. E. Kim et al., *Sci. Rep.***6**, 29472 (2016).

4. Y. Jang, E. Kim et al., *J. Phys. Chem. Lett*. **8**, 364 (2017).

12:00pm **EM-WeM13 Electrically Detected Magnetic Resonance Study of the Relationship Between Silicon Nitride Stoichiometries and Defect Structure and Energy Levels**, ***Ryan Waskiewicz****,* Pennsylvania State University, *M.J. Mutch,* Micron Technology, *P.M. Lenahan,* Pennsylvania State University, *S.W. King,* Intel Corporation

Leakage currents in dielectric thin films utilized in present day integrated circuitry are important reliability concerns. Among the most important dielectric materials are amorphous hydrogenated silicon nitrides (a-SiN:H). These relatively high dielectric constant materials are utilized in many applications such as a passivating layer, an etch stop layer, a diffusion barrier to water, and a gate dielectric. Electron paramagnetic resonance (EPR) studies of a-SiN:H films have identified the K center (a silicon dangling bond back-bonded to three nitrogen atoms) as the single dominating paramagnetic defect in stoichiometric films. Previous studies of spin dependent trap assisted tunneling (SDTAT) detected via electrically detected magnetic resonance (EDMR) provide us with energy levels for these K center defects. [1] However, the effects of varying N/Si stoichiometry on defect levels and defect chemistry have not been studied with EDMR. We have initiated such an EDMR study of SDTAT in a-SiN:H dielectric samples of several stoichiometries.

In our SDTAT/EDMR measurements, a slowly varying magnetic field and an oscillating rf or microwave frequency magnetic field are applied to the thin film samples. As in conventional EPR, energy is absorbed by paramagnetic sites when the resonance condition is met. In the simplest cases, this condition may be expressed by hv=guB, where *h* is Planck's constant, g is an orientation dependent parameter often close to 2, u is the Bohr magneton, and B is the magnetic field. In EDMR, the EPR is detected through a change in current, in our case due to SDTAT.

The devices in our study include 3 nm a-SiN:H stoichiometric samples, and 25 nm a-SiN:H samples with three N/Si ratios of 1, 1.35, and 1.5. The overall device structures under observation consist of Ti/a-SiN:H/p-Si capacitors. A comparison of EDMR measurements taken at high field and frequency (X-band frequency ~ 9.75GHz, 3500G) and low field and frequency (frequency ~ 85-350MHz, 30-125G) provide us with information about defect structure. These comparisons allow us to extract information about the g matrix as well as hyperfine interactions. (The g and hyperfine details provide information about defect structure.) A comparison of EDMR measurements under various biasing conditions allow us to approximately determine the energy levels of the defects involved. This energy level and defect structure information

should lead to a better understanding of transport in these technologically important materials.

[1] M.J. Mutch, P.M. Lenahan, and S.W. King, *Appl. Phys. Lett.* **109**(6), 062403 (2016).

Authors Index

Bold page numbers indicate the presenter