Wednesday Afternoon, October 31, 2012

Energy Frontiers Focus Topic
Room: 15 - Session EN+TF-WeA

Thin Films for Energy Applications

Moderator: M. Filler, Georgia Institute of Technology

2:00pm **EN+TF-WeA1 Batteries and Battery Materials by Vapor Deposition**, ***N. Dudney***, Oak Ridge National Laboratory **INVITED**

Although most commercial rechargeable batteries are prepared by bulk and powder processing methods, vapor deposition of materials has led to important advances for fundamental research, for modification of battery materials and interfaces, and also for commercialization of thin film batteries. Each of these areas will be illustrated with our studies of thin film materials for the electrolyte, anode, and cathode components of rechargeable lithium and lithium-ion batteries with both planar and 3-dimensional architectures.

4:00pm **EN+TF-WeA7 Efficient Radiative and Non-Radiative Energy Transfer from Quantum Dots to Silicon Nanomembrane. Evidence of Waveguiding Phenomena**, ***O. Seitz***, *H.M. Nguyen, W. Peng, Yu.N. Gartstein, Y.J. Chabal, A.V. Malko*, University of Texas at Dallas

Nanostructured materials attract a considerable attention as potential candidates for practical photovoltaic (PV) devices. The majority of current hybrid PV architectures are based on charge transfer schemes, which frequently suffer from bad interface quality and poor carrier transport, consequently lowering the light conversion efficiency. An alternative is offered by non-contact *energy transfer*-based hybrid nanostructures, which combine strongly absorbing components, such as inorganic nanocrystal quantum dots (NQDs), and high-mobility semiconductor (SC) layers. It is envisioned that in such hybrid systems, the excitonic energy would be transferred via non-radiative energy transfer (NRET) and radiative (RET) waveguide coupling across the interface with the subsequent separation and transport of charge carriers entirely within the SC-based component. In this talk, we demonstrate the efficient excitonic sensitization of crystalline Si nanomembranes via combined effects of radiative (RET) and non-radiative (NRET) energy transfer from a proximal monolayer of colloidal semiconductor nanocrystals. Ultrathin, 25–300 nm Si films are prepared on top of insulating SiO_2 substrates and grafted with a monolayer of CdSe/ZnS nanocrystals via carboxy-alkyl chain linkers. The wet chemical preparation ensures that Si surfaces are fully passivated with a negligible number of non-radiative surface state defects and that the separation between nanocrystals and Si is tightly controlled. Combining atomic force microscopy (AFM), ellipsometry, time-resolved photoluminescence measurements and theoretical modeling, we could identify and quantify the individual contributions from RET and NRET, which all combined exceed 85% efficiency of energy transferred into the Si substrate when the nanocrystals are at about 4 nm from the interface. This demonstration supports the feasibility of an advanced thin-film hybrid solar cell concept that relies on energy transfer between strong light absorbers and adjacent high-mobility Si layers.

4:40pm **EN+TF-WeA9 Synthesis of a Thin-Film Yttria-Stabilized-Zirconia (Y_2O_3-ZrO_2) Thin Films by Radical Enhanced Atomic Layer Deposition for µ-Solid Oxide Fuel Cell Applications**, ***J. Cho***, *D. Membreno, B. Dunn, J.P. Chang*, University of California, Los Angeles

Solid Oxide Fuel Cells (SOFCs) is one outstanding alternative energy devices, owing to its significantly higher fuel conversion efficiency than that of fossil fuel based ones while being more environmentally benign. Despite its tremendous advantages and potentials, however, the commercial applications of this technology have been restrained due to its intrinsic problems such as the use of expensive interconnectors and long start-up time, which are inevitably tied to its high operation temperatures (650-1000°C) to maintain high ionic conductivity of electrolytes. To fully utilize the revolutionary potentials of SOFCs in commercial applications, it is imperative to lower its operation temperatures to intermediate temperatures, below 700°C without sacrificing the efficiency of the cell.

Yttria-Stabilized-Zirconia (YSZ, (Y2O3)x-(ZrO2)(1-x)) has been implemented as the electrolyte material of choice in SOFCs because of their high structural, chemical stability with along with high ionic conductivity at the operation temperatures of the cell. While the temperature of the cell could not be lowered as it compromises its conductivity, recent pioneering studies of YSZ in nanoscales have reported significantly enhanced ionic conductivities which could not only lower the working temperature of the cell much below 700°C, but will also allow an expansion in their potential applications even to power portable electronics, resulting in strong scientific and technological interests in investigating the feasibility of developing YSZ in nanoscale for electrolyte applications in next-generation SOFCs, including µ-SOFCs for portable electronics. A thin-film YSZ has been synthesized by Radical Enhanced Atomic Layer Deposition (REALD), with thickness and composition controllability. The metal precursors, Tris(2,2,6,6-tetramethyl-3,5-heptanedionato)yttrium(III) [Y(tmhd)3] and Bis(cyclopentadienyl)dimethylzirconium [Cp2Zr(CH3)2] with Oxygen radicals as oxidant, were used to deposit Y2O3 and ZrO2 with the deposition rates of 0.47 Å/cycle and 0.62 Å/cycle, respectively at ~250°C. The composition of each metal cations in YSZ thin films synthesized as a solid solution of Y2O3-ZrO2 was found to correlate closely to the number of ALD cycles of each constituent oxide. The crystalline structures as well as the local environment of the deposited YSZ thin films were studied by X-ray diffraction (XRD) and Extended X-ray absorption fine structure (EXAFS). The conductivities of REALD YSZ films were found to be both a function of the thickness of YSZ film and the yttrium content in the film. The presence of conductivity enhancement effect on YSZ-SrTiO3 nanoparticles are investigated as well.

5:00pm **EN+TF-WeA10 ALD-enabled Tunneling and Transparent Conductive Oxide Layers for Novel Silicon Nanowire Solar Cells**, *M. Toivola*, Picosun, Finland, ***C.L. Dezelah***, Picosun USA, LLC

In order to enable more efficient harvesting of solar energy in the future, the recently ended (Dec 2011) EU 7th FP project ROD-SOL has successfully developed a novel, high efficiency solar cell based on Si nanostructures. The photoactive layer of this solar cell is a dense "forest" of adjacent Si nanowires (SiNW) deposited on metal or glass substrates. The 3D nanostructure of the NW forests offers various benefits over planar cell geometry, namely, more efficient light absorption due to light scattering in the NW forest, i.e. the NWs work as a light-trapping, antireflective layer.

The best solar cells in the project have already reached a promising value of near 10% efficiency and good long term stability. They were prepared with semiconductor-insulator-semiconductor concept, in which a 1-2 nm layer of ALD-deposited Al_2O_3 functions as a tunneling layer for the minority charge carriers between the SiNWs and the current collecting transparent conductive oxide (TCO) layer on the front side of the cell. Due to the high aspect ratio of the SiNWs ALD is the only method with which ultra-thin but highly uniform, conformal and pinhole-free tunneling layers can be coated on them. Also ALD-deposited, few hundreds of nm thick Al-doped ZnO (AZO) layer works as the TCO in SiNW solar cells, and we have investigated and optimized the electrical and optical properties of these layers.

AZO layers were prepared from trimethyl aluminum (TMA), diethyl zinc (DEZ) and deionized water (DIW). The varied parameters in AZO layers were deposition temperature (100 - 250 ^{o}C) and the percentage of Al in the ZnO matrix (0 - 11 %). The effects of post-ALD annealing and different TMA/DEZ/DIW pulsing orders were also tested.

The best conductivity (1-2 * 10^{-3} Ωm specific resistance) was achieved at 200 ^{o}C with a pulsing ratio of 5 % TMA and 95 % DEZ, equaling ~2 % elemental Al in ZnO. Reverse pulse order, i.e. starting the process with oxidant pulse instead of metal precursor, didn't result in significant performance improvement, neither did the annealing.

Optically, the ALD AZO films had high transparency over the visible wavelengths (no significant dependence on deposition temperature and/or Al doping-%) and refractive index 1.8 – 2, so the films work efficiently as conformal antireflective coatings on Si.

In short, ALD-deposited TCO layers offer a potential alternative to indium-doped tin oxide (ITO) and other scarce element containing TCO materials in solar cells. In the novel nanostructured photovoltaic devices ALD is typically the only method with which thin enough coatings of high quality material (i.e. dense, uniform, conformal, crack- and pinhole-free) can be deposited.

5:20pm **EN+TF-WeA11 Effect of Top Electrodes on the Photovoltaic Properties of Ferroelectric PLZT Thin Film Capacitors**, *V. Nampoori*, ***S. Kotru***, The University of Alabama

Ferroelectrics are emerging as potential candidate materials for energy harvesting and storage. A recent report suggesting the possibility of above band gap voltages from ferroelectric materials has attracted the interest of research community to study these materials for the applications towards non-conventional solar cells devices. Although these ferroelectric solar cells materials do not exhibit very high conversion efficiency compared to the conventional solar devices, but the control of the PV characteristics with controlled polarization in these materials, gives it an edge over the semi-conducting counterparts. It is now, widely agreed that the PV effect in a ferroelectric material is induced by internal polarization of the material

which in turn separates the photo generated electron-hole pairs. However apart from controlling the polarization of the material, there are various other factors which could contribute to the PV output, choice of electrodes, is one among them.

In this work, PV response of ferroelectric PLZT thin film capacitors was investigated. The films were prepared using chemical solution deposition process. Capacitor type solar cells were fabricated from these films using various top electrodes. The IV curves were measured for each device. The ferroelectric/metal barrier as well as the bulk depolarizing field was shown to influence IV characteristics. Use of a metal top electrode with lower work function was found to increase the open circuit voltage (V_{oc}) from 0.17 V to 0.37 V. It was seen that use of a transparent conducting electrode could increase the V_{oc} further to ~ 1.3V. This in turn resulted in enhancement of PV efficiency of the devices. Such increase is attributed from the contribution of ferroelectric/metal barrier rather than from the bulk ferroelectric. These results indicate that choosing an appropriate top electrode can result in significant increase in the efficiency of the ferroelectric photovoltaic devices.

5:40pm **EN+TF-WeA12 Synthesis of Nano-structured Zn_3P_2 as a Solar Cell Absorber**, ***P.S. Vasekar***, *S.P. Adusumilli, D. Vanhart, T. Dhakal*, Binghamton University

With rise in the prices and non-abundance of the materials like indium and gallium current research trends in thin film solar cells have been moving toward development of earth-abundant solar cell materials which can be synthesized using low-cost processes. Also zinc based hetero-junction partners are getting preference over toxic cadmium based compounds such as cadmium sulfide. Zn_3P_2 is alsoan important semiconductor from the II-V group and is used for optoelectronic applications. Zinc phosphide exhibits favorable optoelectronic properties such as direct bandgap of 1.5 eV which corresponds to the optimum solar energy conversion range. Also zinc phosphide has a large optical absorption coefficient of $>10^4$ cm^{-1} , hence it can be positively used as a p-type absorber . Also due to its long minority diffusion length of ~10 μm, high current collection efficiency can be yielded. Zinc and phosphorous are quite abundant in earth's crust. It makes their cost-effective development quite feasible when it comes to large scale production. We have developed a very simple process using chemical reflux technique with Tri-octyl-phosphine (TOP) as a source of phosphorous. Zn_3P_2 has been synthesized in both nanowire and bulk form on zinc foil as well as glass substrates and initial results are quite encouraging. It has been observed that depending on the exposure method with TOP, either nanowire or bulk phase forms. Zinc metal when in contact with liquid TOP, develops nanowires in the range of 50-100 nm and the formation of nanowires exhibits a solution-liquid-solid (SLS) mechanism at the reaction temperature around 350 °C. To the best of our knowledge, zinc phosphide nanowire formation at this low temperature has been observed for the first time. Analysis has been carried out using SEM, XRD, TEM, XPS and PL.

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