

Tuesday Morning, November 10, 2009

Electronic Materials and Processing

Room: A8 - Session EM1+PV-TuM

High Efficiency and Quantum Structure Photovoltaics

Moderator: C.S. Ferekides, University of South Florida

8:00am **EM1+PV-TuM1 Enhancement of the Thermoelectric Figure of Merit in Bulk Semiconductors at the Atomic Level, J.P. Heremans, The Ohio State University** **INVITED**

Recently, several thermoelectric semiconductor systems have been developed with double the thermoelectric figure of merit, zT , of conventional materials. Almost all the progress comes from achieving reductions in thermal conductivity using nanotechnologies or structural disorder. Because the lattice thermal conductivity has a lower limit, the amorphous limit, further progress must come from an enhancement of the electrical properties, in particular the thermoelectric power or Seebeck coefficient. We present a new technique to achieve that, based on creating distortions of the density-of-states by doping with resonant impurities, resulting in a doubling of the zT of PbTe, a semiconductor used for power generation applications near 500 °C. We will also review current progress with this technique in Bi₂Te₃, the other classical thermoelectric, which we study because the commercial materials used for Peltier cooling are (Bi_{1-x}Sb_x)₂(Te_{1-y}Se_y)₃ alloys. The theory behind this approach will be outlined, and its applicability to a wide variety of thermoelectric semiconductors discussed.

8:40am **EM1+PV-TuM3 Synthesis of PbTe Nanowires by Lithographically Patterned Nanowire Electrodeposition (LPNE) and Their Thermoelectric Properties, Y. Yang, D.K. Taggart, R.M. Penner, S.C. Kung, F. Yang, C.X. Xiang, M.A. Brown, J.C. Hemminger, University of California, Irvine**

Thermoelectric materials have received renewed interest in the past decade stemming from theoretical calculations that one-dimensional thermoelectric materials (i.e., nanowires) should show a remarkable enhancement in the dimensionless figure of merit— ZT caused by enhanced Seebeck coefficients, electrical conductivities and/or depressed thermal conductivities relative to their bulk counterparts. The prediction has been verified recently on silicon single-crystalline nanowire-arrays that showed almost one hundred times of enhancement of ZT . In contrast, there has not been any demonstration of a similar effect on PbTe nanowires—one of the best thermoelectric materials in bulk. This presentation reports a synthesis method called lithographically patterned nanowire electrodeposition (LPNE) for making PbTe nanowires and characterization of their thermoelectric properties. The nanowires are semi-rectangular in cross-section with width and height independently controlled from 60 to 500 nm and from 10 to 100nm respectively, and they are electrically continuous up to millimeters. The structure and chemical composition of the nanowires are characterized with X-ray diffraction (XRD), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). The electrical conductivity and Seebeck coefficient are measured at variable temperatures. A method for making suspended nanowires cross an air gap is also developed, which is crucial for measurement of thermal conductivity. Ag-doped PbTe nanowires synthesized by the same method demonstrate tunable thermoelectric

properties due to the modification of the carrier type and concentration.

9:00am **EM1+PV-TuM4 PbSe Quantum-Dot Solar Cells, K.S. Leschkies, T.J. Beatty, M.S. Kang, D.J. Norris, E.S. Aydil, University of Minnesota**

Quantum confinement of electrons and holes in nanometer size crystals (quantum dots or QDs), endows them with properties that may be advantageous for efficient solar-to-electric energy conversion. First, electronic energy levels and optical absorption in QDs can be manipulated by changing their size. This allows the optimization of their optical absorption for maximum overlap with the solar spectrum. Second, the ability to manipulate energy levels through size raises the possibility to make inexpensive multijunction solar cells by judiciously layering different size QDs. Third, it has been suggested that quantum confinement may slow energy dissipative electron and hole relaxation rates such that two new physical processes, multiple exciton generation and hot electron extraction may now compete with relaxation and lead to higher photocurrents or higher photovoltages, respectively. Finally, QDs can be prepared in large quantities as stable colloidal solutions under mild conditions and deposited on surfaces of various planar or nanostructured substrates as thin films through inexpensive high-throughput coating processes to form

photovoltaic devices. For these reasons, solar cells based on QDs may have the potential to achieve high power conversion efficiencies at low cost and are promising candidates for third generation photovoltaic devices. We report a new type of solar cell based on heterojunctions between PbSe QDs and thin ZnO films. We find that the photovoltage depends on the QD size and increases linearly with the QD effective band gap energy. Thus, our solar cells resemble traditional photovoltaic devices based on a semiconductor-semiconductor heterojunction but with the important difference that changing the size of the QDs can vary the band gap of one of the semiconductors and hence the cell's photovoltage. Under simulated 100 mW/cm² AM1.5 illumination, these QD solar cells exhibit short-circuit currents as high as 15 mA/cm² and open-circuit voltages up to 0.45 V. Overall power conversion efficiency of the best device to date is 1.6% but may be increased further using nanostructured interfaces between PbSe QDs and ZnO. Moreover, we show evidence that this new solar cell may be operating like an excitonic solar cell rather than a traditional p-n junction solar cell.

9:20am **EM1+PV-TuM5 Phosphonate Self-Assembled Monolayers as Organic Linkers in Quantum Dot Sensitized Solar Cells, P. Ardalani, T.P. Brennan, S.F. Bent, Stanford University**

Narrow band gap nanostructures such as cadmium sulfide quantum dots (QDs) are known to show size quantization effects as well as multiple exciton generation. They are therefore beneficial for absorption of light in the visible and near infrared region of the solar spectrum and can be used to fabricate photovoltaic devices with high theoretical efficiencies. In quantum dot sensitized solar cells (QDSSCs), these QDs can be engineered to transfer the electron to a wide band gap semiconductor such as titanium dioxide (TiO₂). However, performance in such devices is reduced by charge recombination at the TiO₂ surface and hence use of organic linkers and electron conductors such as self-assembled monolayers (SAMs) on these devices could provide a means of eliminating recombination sites and lead to increased efficiency. In this study, we investigated the effects of different aliphatic and aromatic SAMs with phosphonic acid headgroups and varied tailgroups on the bonding and performance of cadmium sulfide (CdS) QDSSCs. Our studies focus on bonding of the CdS QDs on both planar and nanoporous TiO₂ with or without the SAM linkers. To study the SAM/QD growth on planar surfaces, TiO₂ was deposited on Piranha-cleaned Si or microscope glass via atomic layer deposition (ALD) and the resulting surfaces were characterized by X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), scanning electron microscopy (SEM), and atomic force microscopy (AFM). Next, different SAMs were attached to the TiO₂ substrates from solution, where the effects of chain length, aromaticity, tailgroup, solvent, and dip time on the quality of the SAMs were investigated by the same techniques as well as infrared (IR) spectroscopy, water contact angle (WCA) measurements, and ellipsometry. Finally, CdS QDs were grown on the SAM-passivated TiO₂ surfaces by the successive ionic layer adsorption and reaction (SILAR) process, and the bonding and performance of the resulting materials were evaluated by UV-visible and other spectroscopic techniques. The results were compared to the case of QDs grown on the non-passivated TiO₂ surfaces. Our results show promising differences in the bonding of the CdS QDs at the TiO₂ surfaces with the SAM linkers. We will also present results on the dependence of solar cell performance on the properties of the SAM.

10:40am **EM1+PV-TuM9 High Efficiency Multijunction Solar Cells – Present Status and Future Directions, P. Sharps, Emcore Corporation** **INVITED**

Multi-junction solar cells based on the GaInP₂/GaAs/Ge triple junction architecture have achieved the highest efficiency of any photovoltaic device, for either space or terrestrial applications. However, the cost of these cells is high compared to other photovoltaic devices. For space applications (i.e., satellite power) the higher efficiencies are more critical than cell cost, and on a system level, including launch and deployment costs, the multi-junction cells are actually lower on a \$/watt basis than Si solar cells. The high efficiency multi-junction cell is now widely used on satellites. For terrestrial applications, the high efficiency cells must be used in high concentration systems where the high cell cost is offset by the lower costs of lenses, mirrors, and structure metal. The cell becomes such a small part of the system cost that a doubling of cell cost has a small effect on the cost of power generation. However, the efficiency of the cell may have a much larger effect on the cost of power generated. So for either space or terrestrial applications the efficiency of the photovoltaic device is very important.

Multi-junction solar cells offer a performance advantage over single junction solar cells because of the reduction in carrier thermalization losses. Different parts of the solar spectrum are absorbed by different band

gap materials. III-V materials are able to achieve very high performance on a single junction basis, and when appropriately combined provide an even higher performance advantage. Fortunately, GaInP₂, GaAs, and Ge junctions can be combined in a lattice matched configuration, making a monolithic device with a good combination of junctions for converting the solar spectrum into power. Appropriate modifications can be made to the device to optimize it for either space or terrestrial applications.

To achieve even higher efficiencies, more junctions need to be added and/or the junctions need to be better matched to the solar spectrum. A number of approaches have been studied, including novel materials (e.g., InGaAsN, ZnGeAs₂, etc.), mechanically stacked devices, and metamorphic devices. With metamorphic devices junctions are grown lattice mismatched on one another to achieve the optimal set of band gaps in a complete device. One metamorphic approach, the inverted metamorphic multi-junction (IMM) solar cell, has demonstrated significant performance improvements over the lattice matched triple junction device.

We report on these improvements, describing how the IMM approach is enabling for both space and terrestrial power generation.

11:20am **EM1+PV-TuM11 GaAs Integration on High-Quality Ge on Si for Multijunction Solar Cells**, *D. Leonhardt, J. Sheng*, University of New Mexico, *J.G. Cederberg, M.S. Carroll*, Sandia National Laboratories, *S.M. Han*, University of New Mexico

In an effort to reduce the cost of multijunction solar cells, we have scaled up a process to produce low-defect-density Ge films on 2-inch-diameter Si substrates. These engineered substrates could replace Ge wafers that are currently used in multijunction solar cell fabrication if the Ge film quality on engineered substrates can match that of commercially available epitaxial Ge wafers. We will present results for the scaled up process of engineered Ge on Si substrates, including key aspects of nucleation, defect formation, and defect reduction/elimination, using a variety of characterization techniques. For ensuing GaAs growth, we polish the Ge surface, using a slurry-free H₂O₂ based chemical-mechanical planarization (CMP) process. This CMP technique results in a root mean square (RMS) roughness less than 1 nanometer as revealed by atomic force microscopy. However, stacking faults in the Ge film that terminate at the film surface show up as raised lines after polishing. We have found that thermal annealing at a very early stage of Ge film growth largely eliminates these stacking faults and produces much smoother films than those grown without the annealing step. We have used a combination of atomic force microscopy and transmission electron microscopy (TEM) to investigate the effect of annealing on eliminating the stacking faults and on the initial Ge island morphology. In addition to defect reduction, we have developed a process for cleaning and passivating the Ge surface in preparation for GaAs growth. GaAs films grown on our engineered substrates have an RMS value of 3.6 nm and show integrated photoluminescence intensity that matches GaAs grown on commercially available off-cut Ge substrates. Future work and directions will be discussed in light of our findings.

11:40am **EM1+PV-TuM12 Investigation of Rare Earth - Doped Silicon Nitride Layers for Solar Cell Applications**, *M.C. Petcu, A. Sarkar, M. Creatore, H.T. Hintzen, M.C.M. van de Sanden*, Eindhoven University of Technology, The Netherlands

Nowadays the application of thin SiN_x layers as bulk passivating and antireflection coatings for Si-based solar cells applications is considered to be a successful solution for the increase in efficiency¹. A new concept to further increase the efficiency of the solar cell is based on the light conversion mechanism: according to this approach the solar spectrum can be efficiently modified by shifting the photons towards a wavelength range where the solar cell has a better or higher response².

Recently, a novel class of rare earth (RE)-doped SiN_x layers has been demonstrated to be a highly promising red-emitting conversion phosphor for white-LED applications. These materials have allowed the shifting of the emission wavelength by tuning the concentration of a specific RE element in a SiN_x based crystalline matrix³. The investigation of RE-doped amorphous silicon nitride (SiN_x) compounds, where the electronic properties of Si are combined with the optical properties of RE³⁺ ions, have been shown already potential in optoelectronics⁴. Therefore, parallel studies on the incorporation of a RE material in amorphous SiN_x host lattices, which could be implemented in solar cells to increase the efficiency, are considered to be presently a challenge.

In this contribution the properties of europium- and samarium-doped amorphous SiN_x layers are investigated. The RE-doped SiN_x layers are deposited using a remote PECVD expanding thermal plasma fed with Ar/SiH₄/NH₃ mixtures in combination with a RE magnetron sputtering source implemented in the proximity of the substrate holder. Growth rates of the RE doped layers obtained from Spectroscopic Ellipsometry (SE) measurements were in the range 0.6-2.2 nm/s. The successful incorporation of RE in the SiN_x matrix has been demonstrated by means of Rutherford

Back Scattering (RBS) and X-ray Photoelectron Spectroscopy (XPS) analysis, i.e. up to 2%. Preliminary photoluminescence results point out a broad band emission in the region of 500-800 nm when excitation wavelengths of 270 nm and 320 nm have been used. The emission band observed can be attributed to Sm²⁺.

[1] J. Hong *et al.*, *J. Vac. Sci. Technol. B* 21 (5).

[2] C. Strümpel *et al.*, *Sol. Energ. Mat. Sol. C* 91 (2007) 238 – 249.

[3] Y. Q. Li *et al.*, *J. Alloys. and Comp.* 417, 273 – 279.

[4] A. R. Zanatta, *et al.*, *J. Phys.:Condens. Matter* 19 (2007) 436230.

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