

Wednesday Afternoon, October 17, 2007

Renewable Energy Science & Technology Topical Conference

Room: 602/603 - Session EN+TF+SS-WeA

Photovoltaics, Fuel Cells, and Alternative Energy Materials and Applications

Moderator: J.S. Lewis, RTI International

1:40pm **EN+TF+SS-WeA1 ENABLE-based Low Temperature Growth of In-rich InGaN Films**, *T.L. Williamson, M.A. Hoffbauer*, Los Alamos National Laboratory, *N. Miller, R.E. Jones, K.M. Yu*, Lawrence Berkeley National Laboratory, *P. Flanigan, J. Wu*, University of California, Berkeley, *J.W. Ager, Z. Liliental-Weber, E.E. Haller, W. Walukiewicz*, Lawrence Berkeley National Laboratory

The different optimum growth temperatures for the group III-nitride compounds (e.g. GaN >900C and InN ~550C) make the growth of In-rich and fully compositionally graded InGaN films by MOCVD or MBE a considerable technological challenge. Recently, energetic neutral atomic-beam lithography & epitaxy (ENABLE) has been developed at LANL that makes possible isothermal low-temperature growth of high-quality GaN and $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys over the entire composition range ($0 < x < 1$). ENABLE uses a large flux of neutral nitrogen atoms to activate surface chemical reactions, thereby mitigating the need for high substrate temperatures and allowing the growth of high quality III-nitrides at substrate temperatures far below those of other conventional techniques (<600C) at rates exceeding 2 microns/hr. We will present recent results for ENABLE-grown InN and In-rich InGaN showing spectroscopic, X-ray diffraction, Rutherford backscattering spectrometry (RBS), transmission electron microscopy, and Hall effect measurements to assess the thickness, composition, crystalline quality, and optical and electrical properties of the films. InN films show intense luminescence at the bandgap of ~0.7 eV with electron mobilities exceeding $700 \text{ cm}^2/\text{V}\cdot\text{sec}$. We will also present characterization results for compositionally graded films grown from pure GaN and grading to InN and from pure InN and grading to GaN. These results establish ENABLE as a new technique uniquely capable of growing InGaN films of widely varying composition including compositionally graded InGaN films and InN/GaN heterostructures.

2:00pm **EN+TF+SS-WeA2 Tandem-Junction Solar Cells using BeTe Buffer Layers for AlGaAs Molecular Beam Epitaxy on Silicon Substrates**, *K.P. Clark, E. Maldonado, F. Amir, W.P. Kirk*, University of Texas at Arlington

Monolithically-stacked tandem-junctions allow solar cells with conversion efficiencies above the single-junction limit. An optimal bandgap combination of 1.7 eV and 1.1 eV has a theoretical efficiency above 30% for a series-connected cell. Aluminum gallium arsenide epitaxially grown on silicon is a natural implementation, but has long-standing crystal-quality challenges due to lattice mismatch, thermal expansion mismatch, and island growth of AlGaAs. We report investigations of AlGaAs molecular beam epitaxy on prelayers of the wide-bandgap II-VI compound beryllium telluride BeTe on arsenic-passivated silicon. AlGaAs is nearly lattice matched to BeTe but has a strong tendency for island formation, which is suppressed by low-temperature growth initiation. $\text{Al}_{0.15}\text{Ga}_{0.85}\text{As}$ -GaAs multiple quantum-well p-i-n junction structures were processed and characterized electrically under illumination. The short-circuit photocurrent J_{SC} and open-circuit voltage V_{OC} for the Si/BeTe based junction approach within 15% and 30% respectively of those for a similar junction grown on a GaAs substrate. We report techniques for initial AlGaAs growth including solid-phase epitaxy, BeTe termination, and germanium adlayers studied using RHEED diffraction, X-ray diffraction, and transmission electron microscopy.

Supported in part by NASA.

2:20pm **EN+TF+SS-WeA3 Gaseous Deposition of Lead Sulfide Nanoparticle/Ti-Phthalocyanine Composite Films**, *I.L. Bolotin, D.J. Asunskis, A.M. Zachary, A.T. Wroble, L. Hanley*, University of Illinois at Chicago

Composite materials composed of inorganic semiconductor nanoparticles (NPs) dispersed in organic matrices may find use in photovoltaics, photodiodes, nonlinear optical devices, and other applications. This interest arises from the possibility of tuning the optoelectronic properties of the composite by varying the NP size and concentration within the organic

matrix. Bulk PbS is a group IV-VI semiconductor with a narrow band gap of 0.41 eV at room temperature. Strong quantum size effects occur for <20 nm PbS NPs. Among the other potential advantages of PbS NPs is their high electron affinity, which will enhance charge transfer from an intermingled organic phase. Most of the lead salt NP photovoltaics devices produced to date have been prepared from the solution phase using colloidal techniques. However, gaseous deposition techniques possess certain advantages for the synthesis of nanocomposites: it is inherently suited to film deposition, is compatible with traditional methods of fabricating semiconductor devices, allows control of oxidation during deposition, and it can reduce the agglomeration of NPs. This work demonstrates that gaseous deposition can synthesize a composite film with <5 nm diameter PbS NPs of narrow size distribution embedded within a titanyl phthalocyanine (TiPc) organic matrix. Composite film samples were fabricated here using a cluster beam deposition source combining magnetron DC-sputtering and gas-agglomeration techniques in a fashion similar to that originally developed by Haberland and coworkers. X-ray photoelectron spectroscopy showed that PbS was successfully incorporated into the TiPc matrix during co-deposition. Transmission electron microscopy (TEM) was used to measure the size, shape, distribution, and crystallinity of the NPs in these composite films. Soft-landing of PbS clusters into the TiPc organic matrix allowed the clusters to maintain their three-dimensional structure upon deposition. In the absence of the TiPc matrix, PbS showed the aggregation into much larger, irregularly-shaped particles. PbS NPs appeared homogeneously distributed in the TiPc matrix, with particle spacings of several times the particle diameter. TEM also showed that at least some NPs deposited into TiPc were crystalline. This method also allows for deposition of composite films composed of any evaporable organic and inorganic nanoparticles that can be formed by sputtering and reaction within the cluster source.

2:40pm **EN+TF+SS-WeA4 Plastic Bulk-Heterojunction Solar Cells and Near-Infrared Photodetectors**, *G. Li, Y. Yao*, University of California, Los Angeles, *L. Yu, Y. Liang, S. Xiao*, University of Chicago, **Y. Yang**, University of California, Los Angeles **INVITED**

Polymer based solar cells and photodetectors have tremendous application in harnessing solar energy and photodetection in a cost-effective way. Here we studied the self-organization effect in polymer solar cells and first demonstrated plastic near-infrared photodetectors using low band-gap polymer. The self-organization effect in polymer solar cells based on regioregular poly(3-hexylthiophene) (RR-P3HT):[6,6]-phenyl-C61-butyric acid methyl ester (PCBM) is studied in an evolutionary way, with the difference being spin-coating time t_s (20 to 80 sec) which controls solvent annealing time (t_a) by the solvent residue. Photoluminescence (PL), ultraviolet-visible (UV-vis) absorption spectroscopy, scanning atomic force microscopy (AFM), and grazing-incidence X-ray diffraction (GIXD) were conducted on these blend films and linked to the device performance. In addition to the high performance polymer solar cells, we also demonstrated a fast response near-infrared detector using a new low band gap material. With promising results shown in this presentation, we believe the low band gap materials will open up a new perspective in near-infrared detection.

4:00pm **EN+TF+SS-WeA8 Defect Characterization of CdTe and CdMgTe Solar Cells and Their Correlation to the Device Properties**, *R.G. Dhere, D. Young, J. Scharf, A. Duda, B. To, R. Noufi*, National Renewable Energy Laboratory

CdTe solar cells are at the forefront of commercial thin-film solar cells because of the high laboratory efficiencies and relative ease of fabrication. The current losses for these devices are well understood, with very small room for improvement. On the other hand, open-circuit voltage (V_{oc}) of champion devices is much lower than its potential and presents the only path to improve device performance. In this paper, we present our work on the CdTe and CdMgTe devices fabricated by close-spaced sublimation and physical vapor deposition on glass/SnO₂/CdS substrates. The devices are heat-treated in chloride vapor after deposition, in a controlled ambient, in temperature range of 390°-440°C. The treatment results in recrystallization of the samples deposited at low temperature (~400° C) and selective recrystallization at the CdS/CdTe interface in samples deposited at higher temperatures. The post-deposition treatment also improves the electronic properties of the absorber due to reduced defect density and results in improved device performance. Our investigation studies the effect of bandgap variation and defect density within the space-charge region in the absorber on the device properties, particularly V_{oc} . The bandgap of the alloy is varied by changing the alloy composition of CdS_{1-x}Te_x alloy formed at the CdS/CdTe interface and CdMgTe alloy composition. We examine the bandgap range of 1.45-1.65 eV for the absorber layer. We have varied defect density in the absorber layer by adjusting the substrate temperature and degree of post-deposition chloride treatment. The structural properties

of the samples are studied by atomic force microscopy. The devices have been characterized using drive-level capacitance profiling in combination with capacitance-voltage analysis, in addition to conventional photovoltaic analysis. We will present the data on the devices with a wide range of performance and investigate the correlation between device parameters and the material properties such as bandgap and defect density. This abstract is subject to government rights.

4:20pm EN+TF+SS-WeA9 Electron Backscatter Diffraction of CdTe Thin Films - Effects of CdCl₂ Treatment, H.R. Moutinho, R.G. Dhere, C.-S. Jiang, B. To, M.M. Al-Jassim, National Renewable Energy Laboratory
Electron backscatter diffraction (EBSD) utilizes the electron beam of a scanning electron microscope (SEM) to investigate the crystallographic orientation of materials with high spatial resolution. In EBSD, some of the electrons of the SEM beam are diffracted by the crystalline planes of the sample and collected by a detector, where they form a pattern of Kikuchi lines. These patterns are characteristic of the crystal structure and orientation, and they are collected while the electron beam is being scanned, forming maps of crystallographic orientation. In contrast to X-ray diffraction, which gives the crystallographic orientation of a macroscopic volume of the bulk sample, EBSD provides the individual orientation of volumes with nanometer dimensions. To optimize the EBSD signal, the sample must be inclined by about 70° in relation to the electron beam. Consequently, in rough samples, topographic features shadow some of the diffracted electrons from reaching the detector; thus surface preparation is a common requirement. In this work, we describe the surface processing of CdTe thin films deposited by close-spaced sublimation and physical vapor deposition (PVD). Most of the films studied were too rough to produce good EBSD data. Polishing flattened the sample, but created an amorphous layer on the surface, resulting in no diffraction patterns. Ion-beam milling was not as effective in flattening the surface, but removed rough surface features, resulting in high-quality EBSD data. Etching and light ion milling after polishing also produced good results. After optimizing the sample preparation process, we studied PVD CdTe samples after CdCl₂ treatment using dipping or vapor processes, with different parameters. We observed a striking difference in the sample microstructure depending on the CdCl₂ process and parameters—with grain sizes varying from a few to several dozen micrometers. Our results showed that maintaining a steady source of CdCl₂ during the treatment, compared to a fixed amount, results in completely different recrystallization dynamics. We also studied the grain structure from the substrate to the surface by doing EBSD in cross sections of the samples, as well as analyzing samples after different degrees of polishing.

4:40pm EN+TF+SS-WeA10 Effect of Selenization Temperature on the Grain Growth of Absorber Layer in Ultra Thin CIGS/CdS Solar Cells, S.A. Pette, N.G. Dhere, Florida Solar Energy Center
Solar cells based on CuIn_xGa_{1-x}Se₂(CIGS) have achieved efficiencies of 19.5% and therefore are promising candidates for economic, large-scale production. CIGS thin film solar cells having absorber thickness of 2.5 μm have shown good performance. However, CIGS being a direct bandgap material, theoretically efficient cells could be prepared with absorber thickness as low as 0.5 μm. The rationale behind decreasing the CIGS thickness is to reduce consumption of the scarce and costly resource, indium. It has been observed that the performance of the solar cells degrades as the thickness goes below 0.75 μm. 0.9 μm thick absorber layer are prepared at PV Mat Lab facility at Florida Solar Energy Center (FSEC) with device conversion efficiency of 6.26% as measured at FSEC. The reason for this degradation can be attributed to the defects in the bulk of the absorber material. We know from the Movchan&Demchishin zone model that the rate of grain growth becomes almost negligible once the grains with favored texture and orientation have consumed all the unfavorable grains. This results in columnar grain structure with parallel boundaries. Similar grain structure was observed for the CIGS absorber layers with thickness of about 2.5 μm. It was observed that the grains were finer towards the back contact and larger at the surface and as the thickness goes on reducing there is not enough material for the grains to grow and coalesce. This results in smaller grains and so larger grain boundaries. Another factor affecting the grain size is the mobility of the deposited species which can be increased by increasing the annealing temperatures during selenization. But in case of ultra thin film absorber layer the higher temperatures adversely affect the molybdenum back contact layer thus introducing higher series resistance issues. Hence, in case of ultra thin CIGS absorber layer the selenization time - temperature profile needs to be optimized to obtain a favorable columnar grain structure. The material characterization of the different absorber layers will be carried out using scanning electron microscopy and transmission electron microscopy. The absorber layers would be further fabricated on to complete the device and current-voltage characteristics would be carried out to understand the effect of different temperature-time

profiles on the device parameters such as open circuit voltage, short circuit current, fill factor and finally the conversion efficiency.

5:00pm EN+TF+SS-WeA11 Thin Film Epitaxial Growth of CuInSe₂ Bicrystals for Grain-Boundary Studies, A.J. Hall, D.N. Hebert, A. Rockett, University of Illinois at Urbana-Champaign

Photovoltaics based on CuInSe₂ and related materials have the highest performance of any thin film devices. The nature and role of grain-boundaries in CuInSe₂ devices is currently poorly understood. Previous studies on the influence of grain-boundaries in Cu(In,Ga)Se₂ devices have shown that they exhibit little to no detrimental effect on photovoltaic device performance. Polycrystalline CuInSe₂ devices currently outperform single crystal CuInSe₂ devices. Past studies have been focused on average electrical properties or local surface electrical measurements for observation of the influence of boundaries on film properties. Since polycrystal devices have crystal sizes on the order of 1 micron, optoelectrical measurements are difficult. In order to alleviate these difficulties, a single high-angle grain-boundary in epitaxial CuInSe₂ has been grown on a GaAs bicrystal substrate using a hybrid sputtering and evaporation technique. Electron backscatter diffraction and x-ray diffraction show that film growth is epitaxial across all boundaries (high-angle and twin) in the bicrystal substrates. Atomic force microscopy, profilometry, and focused ion beam cross-sectioning results indicate that surface polarity and termination have a strong influence on film thickness and morphology. Near grain boundary morphology suggests mass transport leading to boundary migration is occurring. It is proposed that high surface energy anisotropy (on the opposing {111}_{A,B} surface facets) motivates mass transport during the growth of CuInSe₂ at crystal boundaries.

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