

Thin Films

Room 306 - Session TF+EM-MoM

Thin Films for Photovoltaic and Energy Applications

Moderator: B.C. Holloway, College of William and Mary

8:20am **TF+EM-MoM1 Hydrogen - The World of Tomorrow?**, *G.N. Richter*, Chevron Fellow Emeritus **INVITED**

We have all heard of the coming world of hydrogen, and how it will become our energy carrier of choice, both clean and efficient, a major input for many chemical processes and, perhaps, our saviour. I am sure that this is coming, and it will bring a major change to many things we do. It will take a revolution to bring this about and it won't be until some time in the future. The question isn't if it will happen, but when will it come and what is needed to bring it about? Others at this meeting are telling us of the uses of hydrogen, its promises and its behaviour. But, there are also important questions to ask about where will the hydrogen come from and the infrastructure needed for us to be able to use it. It is the difficulty in answering these questions that is holding back the revolution. And it is these points that I would like to discuss with you today. Not the promises we have all heard, but how we can get to this "promised" land, as well as some of the things we might all do to get there sooner. What are the needs and opportunities for all of us to address?

9:00am **TF+EM-MoM3 Carbon Nanotube Catalyst for PEM Fuel Cells**, *J. Narayanaamorthy, S. Durairaj, J. Choi*, Wayne State University

Carbon nanotubes have unique properties for future fuel cell applications such as diverse electrical properties, large surface area to volume ratio, chemical inertness, etc. The role of carbon nanotubes for the polymer electrolyte fuel cell has been investigated. First, the morphological, electrical, and mechanical role of the carbon nanotubes in the catalyst layer was studied. There was minimal cracking and maximal interconnect in the layer with carbon nanotubes. The resistance of the catalyst layer reduced due to the presence of carbon nanotubes and mechanical properties also showed good improvement. Further, carbon nanotubes themselves were employed as catalyst in place of noble metals and were optimized by tuning the electronic properties of carbon nanotubes. In this presentation, we will discuss the correlation between catalytic activity and the electronic structure of carbon nanotubes.

9:20am **TF+EM-MoM4 Growth of CIGSS Thin Film Solar Cells on Flexible Stainless Steel Substrates of Various Thicknesses**, *A. Kadam, A. Jahagirdar, N.G. Dhere*, University of Central Florida

The article presents the effect of surface roughness and thicknesses of stainless steel(SS) substrates on the growth behavior of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ (CIGSS) absorber thin film solar cells. The work was carried out on 430 grade SS of thicknesses 25 μm , 50 μm and 127 μm . Surface roughness gradually decreased from 254 \AA for 25 μm to 62.3 \AA for 127 μm substrate. Thinner foil has higher surface roughness as it required more processing steps. Deposition sequence was Mo/SS/Mo/CIGSS/CdS/ $\text{i:ZnO/ZnO:Al/Ni/Al}$. Mo back contact and Cu-Ga-In metallic precursors were deposited by DC magnetron sputtering. Mo was deposited on both the sides of SS to prevent the reaction of selenide and sulfide gases with SS during processing. Mo was deposited in a three-layer sequence. Mo layer deposited at low DC power and high argon gas pressure develops tensile stress while that deposited at high power and low pressure exhibits compressive stress. Tensile layer was sandwiched between two compressive layers to reduce the overall stress and to build the thickness of 500 nm. Identical parameters were used for deposition of metallic precursors on all three substrates. The elemental stack was selenized at 400°C for 10 minutes followed by sulfurization at 475°C for 20 minutes. CdS, n-type hetero-junction partner was deposited by chemical bath deposition. Window bilayer of i:ZnO and ZnO:Al were deposited by RF magnetron sputtering and Ni/Al contact fingers were deposited by e-beam evaporation. The crystal structure, surface morphology, chemical variation and cell efficiency were studied using the characterization technique such as x-ray diffraction, scanning electron microscopy, Auger electron spectroscopy, transmission electron microscopy, current-voltage and quantum efficiency measurement to bring out the variation in the growth behavior and cell efficiency on substrates having varied physical properties.

9:40am **TF+EM-MoM5 Surfactant-assisted Growth of CdS Thin Films for Photovoltaic Applications**, *C.L. Perkins, F.S. Hasoon*, National Renewable Energy Laboratory

A common non-ionic surfactant, Triton X-100, was used to modify the chemical bath deposition (CBD) of CdS "buffer" layers on Cu(In,Ga)Se_2 (CIGS) thin films. X-ray photoelectron spectroscopy and Auger electron spectroscopy data demonstrate that films produced with the surfactant have about the same levels of impurities as films grown without it. It was found that Triton X-100 allowed the use of CdS layers that were 3-4 times thinner than those used normally in high efficiency CIGS-based devices, with no loss in cell performance. For these thin CdS layers and relative to devices made without the surfactant, average absolute cell efficiencies were increased from 10.5% to 14.8%, or by a relative 41%. Visual inspection of the CdS depositions reveals one possible mechanism of the surfactant's effects: bubbles that form and adhere to the CIGS surface during the chemical bath deposition are almost completely eliminated with the addition of the TX-100. Thus, pinholes and thin areas in the CdS layers caused by poor wetting of the substrate surface are sharply reduced, leading to large increases in the open circuit voltage in devices produced with the surfactant.

10:00am **TF+EM-MoM6 Surface Energies and Surface and Grain Boundary Nanochemistry of Cu(In,Ga)Se_2** , *C. Lei, D. Liao, A. Hall, I.M. Robertson, A. Rockett*, University of Illinois

A combination of angle-resolved photoelectron spectroscopy, atomic force microscopy, and analytical high-resolution transmission electron microscopy including nanoprobe energy dispersive spectroscopy (EDS) and angular darkfield imaging have been used to characterize the surfaces and grain boundaries in a wide variety of Cu(In,Ga)Se_2 epitaxial single crystal and polycrystalline thin films. We have observed the formation of a wide variety of nanoscale and microscale voids in polycrystalline grain boundaries and in heteroepitaxial interfaces. It is argued that these are Kirkendall voids. Likewise, trapped internal voids within grains are observed in dislocation cores and at twin termination boundaries. These have been analyzed and a Wulff construction developed to characterize the surface energies in the material. The results show that the polar metal-terminated (112) planes are the lowest energy surfaces, followed by the Se-terminated (112) planes. These results are consistent with the surface morphology of growing epitaxial layers of various orientations, indicating that the surface faceting is a largely equilibrium rather than kinetically-determined result. Other planes are stable when covered by a surfactant layer of Cu_2Se , which occurs naturally when the film is deposited in an average Cu-rich condition. Grain boundaries are also found to exhibit faceted growth. Surprisingly, in spite of these surfaces being polar, no chemistry change is observed with nanoprobe EDS in the grain boundaries relative to the bulk grains for films grown at high temperatures. For low temperature depositions (below 450°C), non-equilibrium grain boundary compositions are observed. Clean metal-terminated (112) surfaces are shown to have Fermi energies higher in the energy gap when treated in various ways than the corresponding Se-terminated surfaces. The results are related to solar-cell device performances, the primary application of these materials.

10:20am **TF+EM-MoM7 Preparation and Characterization of Transparent Conducting ZnTe:Cu Back Contact Interface Layer for CdS/CdTe Solar Cell**, *U. Avachat, N.G. Dhere*, University of Central Florida

This paper presents preparation and characterization of transparent conducting ZnTe:Cu back contact interface layer for CdS/CdTe thin film solar cells for multijunction thin film PV applications. Polycrystalline ZnTe:Cu thin films were grown by Hot Wall Vacuum Evaporation technique. Hot wall set up was developed to obtain highly stoichiometric films with better material yield and thickness uniformity. 500 nm ZnTe:Cu films were prepared on glass and characterized for stoichiometry, structural properties and optical transparency by electron probe microanalysis, optical transmission spectroscopy and X-ray diffraction technique respectively. Highly stoichiometric ZnTe:Cu films were obtained on glass with optical transparency in the range of 70-80 % in near IR region. X-ray diffraction patterns revealed face-centered cubic phase of ZnTe with preferred {111} orientation. CdS/CdTe solar cells were completed with configuration, $\text{CdS/CdTe/ZnTe:Cu/ZnO:Al/Ni-Al}$ and $\text{CdS/CdTe/ZnTe:Cu/ITO/Ni-Al}$. ZnO:Al and ITO thin film layers were deposited by RF magnetron sputtering and Ni-Al contact fingers were deposited by e-beam vacuum evaporation through metallic mask. Completed CdS/CdTe solar cells were characterized for their I-V characteristics using current voltage measurements.

Monday Morning, October 31, 2005

10:40am **TF+EM-MoM8 CuPc:C60 Blend Film: A Photoemission Investigation**, L. *Lozzi*, University of L'Aquila and INFN-CNR, Italy; V. *Granato*, University of L'Aquila, Italy; S. *La Rosa*, Sincrotrone Trieste Scpa, Italy; S. *Santucci*, University of L'Aquila and INFN-CNR, Italy

Recently a strong research effort has been devoted to study the application of organic-inorganic multilayer films for the preparation of photovoltaic devices. Generally these devices are composed by a multilayer of an organic film which is the active layer, a charge acceptor (to reduce the electron-hole recombination probability) and the two metallic contacts to collect the charges (as ITO, Au and Al). The most used compounds are Copper Phthalocyanine (CuPc), as organic layer, and the C60, as electron acceptor. An improved system, showing a higher efficiency, can be prepared depositing, between the metallic contacts, a blend of active layer and charge acceptor. With this design one of the most important parameter, the exciton diffusion length (which is quite small in the organic systems), becomes less important because it is obviously much higher than the CuPc-C60 distance when these molecules are bonded. The realization of these blend films determines the strong reduction of the luminescence of the CuPc film, but it is not clear if in this blend film there is the formation of bonds between CuPc and C60 molecules or if its electronic structure is simply the sum of the electronic states of the two single compounds. In this contribution we will show the results obtained using soft X-ray photoemission spectroscopy on CuPc:C60 blend films, with different concentrations. These films have been deposited in ultra high vacuum by thermal evaporation. We will show a variation of the HOMO states as a function of the concentration ratio. This HOMO level moves towards the Fermi level, influencing the interface properties with the metallic contacts. The intensity and position of this level is strongly influenced by the CuPc:C60 ratio. This result could be related to the variation of the optical properties of these films.

11:00am **TF+EM-MoM9 Silicon Thin Films from Trichlorosilane for Electron Beam Recrystallized Solar Cells**, C. *Groth*, K. *Ong*, Hamburg University of Technology, Germany

The project's aim is to produce polycrystalline thin film solar cells on low cost substrates, especially on float glass. The chemical processing is entirely dry, which leads to high efficiency and throughput. There is no size limitation using this sequence of processing; even the in-line production of complete solar panels is feasible. An intermediate Tungsten (W) layer of approximately 1 μm is used to maintain mechanical stability at high temperatures. Furthermore, it is used as diffusion barrier during the recrystallisation process and serves as back surface reflector and electrical contact. Two deposition processes are currently under investigation: DC-magnetron sputtering and plasma enhanced chemical vapour deposition (PECVD) using tungstenhexafluoride (WF_6) as precursor. Both processes are using substrate temperatures of $\sim 400^\circ\text{C}$. Analysis using XRD (x-ray diffraction) shows formation of $\alpha\text{-W}$ for sputtered layers while PECVD layers consist of $\alpha\text{-W}$ and $\beta\text{-W}$, depending on the process parameters. The silicon (Si) basis with a thickness of 15 μm is deposited by PECVD directly from trichlorosilane (SiHCl_3) as precursor at high rates of $\sim 200\text{ nm/min}$. Substrate temperature during the process is $\sim 550^\circ\text{C}$. RF frequencies of 13.56 MHz are used in both PECVD processes. P-doping of the basis is done in-situ using borontrichloride (BCl_3). The nanocrystalline silicon film is recrystallised by a line-shaped electron beam at high velocities of about 60 mm/s. This leads to grain sizes of up to several 100 μm . A PECVD deposited amorphous silicon layer will be used as hetero emitter to complete the solar cell.

11:20am **TF+EM-MoM10 Plasma-Assisted Co-Evaporation of Thin Films for Photovoltaic Applications**, S. *Kosaraju*, J.A. *Harvey*, C.A. *Wolden*, Colorado School of Mines

This presentation describes the development of plasma-assisted co-evaporation (PACE) and its application to the formation of $\beta\text{-In}_2\text{S}_3$ and InN thin films. The former is an alternative window layer for copper indium diselenide based devices and the latter is a potential absorber. In PACE metals are supplied by conventional thermal evaporation, while the chalcogen or nitrogen gas precursors are activated by an inductively coupled plasma (ICP) source. The performance of the ICP source to activate both H_2S and N_2 was measured and optimized using a combination of optical emission spectroscopy and mass spectrometry. Transport modeling was used to quantify the flux distributions of both the co-evaporated metal and the reactive species from ICP source impinging upon the substrate. The source geometries were positioned asymmetrically so that the influence of composition and absolute rate could be ascertained from a single deposition experiment in a combinatorial approach. Model predictions were compared and validated

using measurements of film thickness, composition, and quality. Through the deposition of $\beta\text{-In}_2\text{S}_3$ and InN it was demonstrated that PACE provides substantial improvements in both materials utilization and substrate temperature reduction. For the case of $\beta\text{-In}_2\text{S}_3$ it was observed that film quality was highly sensitive to the S/In ratio. The buffer layer was formed as low as 100°C , and it was found that both the morphology and optical band gap were strong functions of temperature. In the case of InN the most important parameter was the excitation of nitrogen in the ICP source. It was shown that the introduction of argon was beneficial to nitrogen activation as evidenced by measurements of crystal quality and electronic properties.

11:40am **TF+EM-MoM11 Anomalous High Seebeck Coefficient Observed in V_2O_5 Thin Films**, S. *Iwanaga*, N.T. *Nguyen*, R.B. *Darling*, F.S. *Ohuchi*, University of Washington

Vanadium oxides, especially vanadium pentoxide (V_2O_5), have gained recent attention for a wide range of applications such as ion storage layers in solid-state batteries, windows for photovoltaic cells, and electro- and photo-chromic devices. Various transport properties have been investigated in the past; however, its thermoelectric properties have not been well characterized. Recently, we observed an anomalously high Seebeck coefficient from sol-gel deposited V_2O_5 thin films. Seebeck coefficients of between -500 to -700 $\mu\text{V/K}$ were measured, with corresponding electrical conductivities ranging from 0.005 to 0.1 $\text{ohm}^{-1}\text{cm}^{-1}$. Unlike conventional materials, the Seebeck coefficients and electrical conductivity act in parallel, suggesting that the carrier concentration increases while maintaining a high Seebeck coefficient. This peculiar transport characteristic appears to be related to polaron hopping. The power generation of the film was further estimated by current-voltage (I-V) measurements to assess the thermoelectric performance of the films. The I-V measurements were performed while applying a temperature gradient to the film by applying a current source in such a way that the thermopower current was suppressed by applying the current in the opposite direction. The I-V characteristics at different applied ΔT were thus obtained, from which the output power (load characteristic, P) was calculated from the I-V data.

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