

Thursday Afternoon Poster Sessions

Energy Frontiers Focus Topic

Room: Central Hall - Session EN-ThP

Energy Frontiers Poster Session

EN-ThP1 Tungsten Carbide: Synthesis and Reactivity with Oxygen on the Nanoscale, *J.B. McClimon, P. Reinke*, University of Virginia

Transition metal carbides have shown considerable promise as catalysts, which is often attributed the similarities in electronic structure between noble metals and transition metal carbides. The addition of tungsten carbide to microbial fuel cells, and their use as an anode material has proven to be quite advantageous. However, the bottleneck in the use of tungsten carbide lies in the loss of function due to partial or complete oxidation of the surface. We study the reactivity of tungsten, and carbon-rich tungsten carbide clusters with oxygen to investigate the progression of oxidation. We suggest that carbon-rich carbide surfaces are less susceptible to oxidation and can be regenerated by annealing.

The tungsten and tungsten carbide clusters are made by the co-deposition of W and C₆₀ which enables us to fine-tune composition in a wide range. The morphology and electronic structure of the surface is probed with STM in-situ, which is supplemented by chemical analysis with XPS, and structural analysis with TEM. The progression of oxidation is observed with bandgap maps with spatial resolution in the nm-range. The experiments were performed on graphite substrates, where the metal clusters remain highly mobile and do not react in the temperature regime of our work (< 650 K).

We begin with a discussion of the synthesis of clusters with compositions ranging from pure W-clusters, to carbon-rich surfaces. The cluster sizes are between 5-30 nm, and the carbon is introduced either by co-deposition of W and C₆₀ or by the deposition of fullerenes on pure W-clusters (and vice-versa). The C₆₀ aggregates to large islands and a reaction with the W-clusters is only initiated by annealing, and leads to carbon-terminated metallic clusters. The motion of fullerene molecules is reflected in the sawtooth signature of tip induced displacement, which is also a probe for the surface chemistry. The co-deposition of W and C₆₀ (and W deposition on C₆₀) leads to the formation of spherical structures whose granularity reflects the dimensions of the C₆₀ cage. We assume that the C₆₀ cage reacts with surface W but the low temperature prevents collapse. The oxidation of tungsten clusters has been observed as a function of oxygen partial pressure, and shows the progression of the reaction as a function of cluster size and surface morphology. We will present a complete set of bandgap maps, which are recorded during the oxidation at room temperature and elevated temperature for the different carbide structures. A model describing the oxidation as a function of carbide structure and composition will be presented.

EN-ThP2 F-doped ZnO Thin Films Deposited by Pulse DC Magnetron Sputtering of Zinc Target, *B.-H. Liao*, Instrument Technology Research Center, Taiwan, Republic of China

In this study, Fluorine doped ZnO (FZO) films were deposited on glass substrate by pulse DC magnetron sputtering of zinc targets with Ar, H₂, O₂ and CF₄ containing gas mixtures at room temperature. Increasing CF₄ gas in ZnO films can increase the carrier concentrations but slightly decrease the mobility. After introducing 1 sccm CF₄ gas in ZnO films we can get the lowest resistivity 7.6×10⁻⁴ (Ω-cm) with mobility 12.4 cm²/V-s and carrier concentrations 6.6×10²⁰ cm⁻³. Besides, its average transmittance in the visible region was over 82.95%. All of the results indicate that we have found a cost effective and mass production process suitable for the application of manufacture in the real-world industry.

EN-ThP3 Photoresponse of PbS Nanoparticle - Quaterthiophene Films Prepared by Gaseous Deposition as Probed by XPS, *M. Majeski, D. Pleticha, I. Bolotin, L. Hanley*, University of Illinois at Chicago, *E. Yilmaz, S. Suzer*, Bilkent University, Turkey

Semiconducting lead sulfide (PbS) nanoparticles were cluster beam deposited into evaporated quaterthiophene (4T) organic films, which in some cases were additionally modified by simultaneous 50 eV acetylene ion bombardment. Surface chemistry of these nanocomposite films was first examined using standard X-ray photoelectron spectroscopy (XPS) and laser desorption/ionization mass spectrometry. XPS was also used to probe photoinduced shifts in peak binding energies upon illumination with a CW green laser and the magnitudes of these peak shifts were interpreted as changes in relative photoconductivity. The four types of films examined all displayed photoconductivity: 4T only, 4T with acetylene ions, 4T with PbS nanoparticles, and 4T with both PbS nanoparticles and acetylene ions. Furthermore, the ion-modified films displayed higher photoconductivity,

which was consistent with enhanced bonding within the 4T organic matrix and between 4T and PbS nanoparticles. PbS nanoparticles displayed higher photoconductivity than the 4T component, regardless of ion-modification. Finally, development of a new instrument is discussed that will allow analysis of films without prior exposure to air.

EN-ThP4 The Investigation of the Shunt Resistance using Conductive AFM and EL Measurements in Si Based Thin Film Solar Cells, *M.H. Joo, J.M. Lee, K.H. Park*, LG Electronics Advanced Research Institute, Republic of Korea

Silicon (Si)-based solar cells are of great interest for photovoltaic applications, such as bulk type, thin film type, and heterojunction type. Recently amorphous silicon based thin film solar cells have attracted much attention from researchers and engineers because of low consumption of raw materials and low temperature deposition. However, the conversion efficiency of these solar cells is still very poor compared to other types of solar cells. An improved understanding on defects in Si based thin film solar cells is required to further enhance cell performance. Due to the short exposure time and high spatial resolution, camera-based techniques, such as photoluminescence (PL), electroluminescence (EL) and dark lock-in thermography (DLIT), have recently emerged as powerful characterization tools for the investigation of different loss mechanisms in solar cells and modules. And the combination of these techniques with high resolution electrical and structural analysis such as conductive atomic force microscopy (c-AFM) and transmission microscopy (TEM) allow for advanced studies on shunt and for determination of recombination current.

In this report, we studied the evolution of the shunt resistance in Si based thin film solar cells. The solar cell (1x1 cm²) structures have a configuration of glass/Al-doped ZnO (AZO)/ a-Si/ a-SiGe/Al. AZO and Al are top and bottom electrodes respectively, deposited with DC magnetron sputter. A-Si and a-SiGe are used for absorption layers prepared by plasma enhanced chemical vapor deposition (PE-CVD). AZO was textured for the light management before the deposition of absorption layers. For defect investigation of solar cells, we measured the samples with both EL and c-AFM. Electroluminescence is driven by injecting a constant current from a power source into the cell. After EL measurements, current distributions in the local area of the cells were evaluated with c-AFM. EL results show the recombination loss of defect area, which is correlated with high leakage current area of c-AFM results. In the result of TEM analysis, low shunt area in the cells evolved from the crack defects in absorption layers. The surface structures of AZO such as high angle textures and pinhole defects make an important role of crack evolution in the absorption layers. When the sample was controlled with low angle AZO texture and no pinhole defects, there was no recombination loss and leakage current in the cells.

EN-ThP5 Growth Methods and Applications of SiC Nanopowder and Nanowhiskers, *R. Dhiman*, University of Southern Denmark, *E. Johnson*, University of Copenhagen, Denmark, *P.K. Kristensen*, Aalborg University, Denmark, *P. Morgen*, University of Southern Denmark

Nanomaterials have in a number of cases shown physical and chemical properties differing from their macroscopic counterparts. These differences can be tailored through form and size of the nanostructured materials, related to the restriction of the electronic degrees of freedom in one-, two-, or three dimensions. In this study, nanoporous SiC has been produced through reactions at high temperatures between carbon nanoparticles and SiO gas, while SiC nanowhiskers are made from saw dust impregnated with TEOS, reacting at high temperatures in a complex set of reactions to produce SiC clusters with a high concentration of SiC nanowhiskers sticking out perpendicularly from planar areas on the clusters. After suitable separation and extraction procedures individual crystals or whiskers may be handled and studied, with SEM and TEM methods. The SiC nanopowder is successfully applied as support material for Pt nanoparticles in the fuel cell technology, while the individual whiskers show very interesting mechanical properties and one-dimensional semiconductor properties. They are also currently used, in agglomerate form, as a very stable and inert type of binder material for new water-electrolysis active membrane systems.

EN-ThP6 Epitaxial Growth of ZnInON Films for Piezo-Electric-Field Effect MQW Solar Cells, *K. Matsushima*, Kyushu University, Japan

Multi-quantum well (MQW) solar cells belong to the most promising "third generation photovoltaics" with ultra-high conversion efficiencies at low cost. In order to approach their theoretical maximum efficiency (>50%), a significant improvement in the extraction efficiency of photo-generated carriers is important. We have recently proposed piezo-electric-field effect (PEF) MQW solar cells that utilize novel oxynitride semiconductor ZnInON (ZION) films [1,2]. Our simulation predicts that the electron-hole recombination rate in ZION-QWs is noticeably low compared to those in

conventional QWs with III-V materials such as GaAs and InGaN. Here we fabricate epitaxial ZION films on GaN and ZnO templates aiming at realization of PEF-MQW solar cells. Furthermore, we also demonstrate coherent growth of ZION films in order to study the piezo-electric field in ZION-QWs which can prevent the recombination and thus enhance the extraction efficiency of photo-generated carriers.

Epitaxial ZION films were fabricated by RF magnetron sputtering, which is suitable for large-area and low-cost fabrication. Commercial GaN templates that were fabricated by metal-organic chemical vapor deposition (MOCVD) and sputtered ZnO templates were used as epitaxial substrates. The ZnO templates were fabricated by RF magnetron sputtering at 700°C in Ar-O₂ atmosphere on ZnO buffer layers that were fabricated via nitrogen mediated crystallization (NMC) in N₂-Ar atmosphere at 700°C [3,4]. On GaN and ZnO templates, ZION films were deposited in N₂-Ar atmosphere at the total pressure of 0.2-0.5 Pa. The applied RF power was 10-90 W and the deposition temperature was 400°C. The film thickness was 30-700 nm.

X-ray diffraction measurements show that the ZION films have wurtzite crystal structure and the full width at half maximum (FWHM) of rocking curve from (002) plane for the films is noticeably small of 0.115°, indicating small fluctuation of the crystalline orientation. Furthermore, measurements of reciprocal lattice map of (105) plane suggest that the ZION films are grown coherently on GaN templates, indicating that a piezo-electric field can be generated. From these results, we conclude that ZION films are full of promise for Piezo-Electric-Field effect MQW solar cells that can be fabricated at low cost.

[1] N. Itagaki, *et al.*, Jpn. Patent Application No. 2012-49805 (2012) (in Japanese).

[2] N. Itagaki, *et al.*, U.S. Patent Publication No. 2010/0109002 (2010).

[3] N. Itagaki, *et al.*, Appl. Phys. Express 4 (2011) 011101.

[4] K. Kuwahara, *et al.*, Thin Solid Films 520 (2012) 4674.

EN-ThP7 Texture-Etched Surface Structure Control of Transparent Conductive Impurity-Doped ZnO Films Deposited by r.f. Power Superimposed d.c. Magnetron Sputtering. T. Minami, T. Fujita, T. Miyata, J. Nomoto, Kanazawa Institute of Technology, Japan

This paper describes the influence of the supplied r.f. power on the light scattering characteristics and the surface texture formation obtainable by wet-chemical etching transparent conducting impurity-doped ZnO thin films prepared by an r.f. power superimposed d.c. magnetron sputtering deposition (rf+dc-MSD) using a high-density-sintered rectangular Al- or Ga--doped ZnO (AZO or GZO) target (127 mm×275 mm) : prepared with an Al₂O₃ content of 1 or 2 wt.% or Ga₂O₃ content of 5.7 wt.%, respectively. Both AZO and GZO thin films were prepared with a film thickness of either 1000 or 2000 nm on OA-10 glass substrates at a temperature of 200°C by varying both the supplied d.c. and r.f. power used in the rf+dc-MSD: d.c. power in the range of 0-800 W and r.f. power in the range of 0-1000 W. The surface texture formation was carried out by wet-chemical etching (in a 0.1% HCl solution at 25°C) conducted after heat-treatment with rapid thermal annealing (RTA) at 500 or 550°C for 5 min in air. It was found that the light scattering characteristics and surface texture formation obtainable for texture-etched AZO (or GZO) thin films were considerably dependent on both the ratio of supplied r.f. to d.c. power as well as the Al (or Ga) content doped into the films. In particular, the haze value was significantly improved at wavelengths up to about 1200 nm in the near-infrared region in surface-textured AZO films prepared with an increased ratio of supplied r.f. power to d.c. power and etched after being heat treated with RTA, whereas the film deposition rate was found to decrease with the increased power ratio. The obtained haze value improvement is attributable to an increase of etch pit size as well as a decrease of carrier concentration. In addition, the obtainable improvement in texture-etched AZO thin films was also found to be considerably dependent on the Al content doped into the films. In particular, texture-etched AZO thin films that are appropriate for transparent electrode applications in thin-film solar cells were obtained with the following preparation conditions: rf+dc-MSD using an AZO target with an Al₂O₃ content of 2 rather than 1 wt.%, r.f. power superimposed at an appropriate value and wet-chemical etching after heat-treatment with RTA. A high haze value above 80% at wavelengths up to 1100 nm in the near-infrared region was attained in texture-etched AZO thin films prepared by rf+dc-MSD (700 W r.f. component added to a constant d.c. power of 570 W) using an AZO target with an Al₂O₃ content of 2 wt.%.

EN-ThP8 Thermoelectric Properties of Sb₃ Doped Bi₂Te₃+Bi₂Se₃ Alloys by Mechanical Alloying and Spark Plasma Sintering. M. Babu, S.J. Hong, Kongju National University, Republic of Korea

Thermoelectric (TE) materials and its devices provide attractive increasing attention because of their potential applications in the field of energy conversion, cooling for electronic devices and thermal sensors. For enhancing the thermoelectric performance, we fabricated the micro-sized n-

type Bi₂Te₃+Bi₂Se₃ (Bismuth-Tellurium-Selenium) with different compositions doped with 0.05 wt%SbI₃ alloys via high energy mechanical alloying which is associated with vacuum atmosphere. The milled powder was consolidated by Spark Plasma Sintering (SPS) technique at the temperature range of 400°C with a holding time of 10 minutes at 50 MPa pressure. The effects of milling time and temperatures were investigated. In order to investigate microstructural analysis of the samples, both Optical microscope (OM) and Scanning Electron Microscope (SEM) were used. The phase of different compounds was characterized by X-ray Diffraction (XRD). Mechanical properties were calculated by measuring the density and micro Vickers hardness of the samples. The temperature dependence of the Seebeck coefficient, electrical resistivity and hall coefficient were determined for the alloys samples with different compositions. From the experimental results, the thermoelectric properties are mainly influenced by the milling time, vacuum condition and temperature. The maximum values of Figure-of-merit (ZT) for the different compounds of samples were calculated using the thermoelectric properties.

EN-ThP9 Structure-to-Function Relationship in Porous Pt/TiO₂/Ti Planar Nanostructures with a Potential Barrier for Chemicurrent Related Applications. S. Dasari, M. Ariyan, M. Hashemian, E. Karpov, University of Illinois at Chicago

Recent observations of enhanced chemicurrent effects of heterogeneous reactions on porous MIM structures with an intrinsic potential barrier make them promising for novel sensing and energy conversion applications. This presentation describes relationships between morphological features of Pt/TiO₂/Ti nanostructures, derived from XRD and SEM studied, and chemicurrent production capabilities of this material system. In particular, samples containing anatase phase in the oxide film layer show significantly greater chemicurrent effect of catalytic hydrogen oxidation on the nanostructure surface and chemical to electrical energy conversion efficiency than those with a dominant rutile phase. Strategies of thin oxide film growth by plasma electrolytic oxidation method leading to porous anatase TiO₂ thin films are also presented.

EN-ThP10 Investigation of the Molecular Interaction between CdSe Quantum Dots and P3HT for Hybrid Solar Cell Applications. A.S. Karakoti, P. Nachimuthu, S. Thevuthasan, Pacific Northwest National Laboratory

We took a systematic approach to study the interaction between CdSe quantum dots (QDs) and regioregular P3HT polymer using spectroscopic and imaging tools. Photoluminescence (PL) measurements following the titration of CdSe quantum dots with P3HT showed evidence of charge transfer between the CdSe QDs and the P3HT matrix. The titration led to an immediate quenching of main PL emission from both CdSe and P3HT and a new emission in low energy region of the electromagnetic spectrum starts appearing from the recombination of electrons in CdSe with holes in P3HT. The effect of the size of QDs on charge transfer as a function of reaction time following the addition of CdSe quantum dots in to a fixed concentration of P3HT was monitored. The time course PL measurements show the quenching of main PL emission from P3HT follow the order 6.6 nm<3.3 nm<2.1 nm while no significant changes was observed in the absorbance spectrum. These results suggest that the size-dependent interaction between QDs and P3HT. However, dynamic light scattering measurements (DLS) from the ligand capped CdSe QDs indicate a strong tendency for agglomeration of smaller QDs in the presence of P3HT. Addition of P3HT to a known concentration of CdSe QDs increases their average diameter for 2.1nm and 3.3nm QDs in toluene while the average diameter of QDs with 6.6nm in toluene remains unchanged at the same concentrations. This suggests that the interaction between CdSe QDs and P3HT is controlled by the agglomeration of QDs and not by the size of the dots. Findings from these results and the effect of changing the capping ligands of CdSe QDs on the charge transfer will be discussed.

EN-ThP11 Low-Damage Deposition of Thin Silicon Films for Solar Panel Production using Surface-Wave Plasma Source. J. Peck, University of Illinois at Urbana Champaign, P. Zonooz, Starfire Industries LLC and University of Illinois at Urbana Champaign, D. Curreli, University of Illinois at Urbana Champaign, M. Reilly, R. Stubbers, B. Jurczyk, Starfire Industries, LLC, D.N. Ruzic, University of Illinois at Urbana Champaign

An innovative kind of plasma source for the deposition of thin silicon films used in semiconductor manufacturing is currently under development at Starfire Industries LLC and CPMI Center for Plasma Material Interaction, University of Illinois Urbana Champaign. The source, operating in the microwave range, is able to efficiently generate high-density and low-electron-temperature SiH₄-H₂ plasmas, and can easily be scaled upward to the deposition of thin films on large-area surfaces. The silicon films deposited at low RF power on glass substrates have been characterized using multiple techniques, comprising SEM, Ellipsometry and Raman

Spectroscopy. Spectroscopic data in the UV-VIS-NIR range have been acquired during the discharge operations for plasma characterization. By using Raman spectroscopy, the crystalline volume fraction of the deposited films has been obtained for several input mass-flows of silane, as a function of the substrate temperature and for several pressures of the Hydrogen gas. The averaged film growth rate has been obtained from both ellipsometry measurements and SEM imaging. From the results of the preliminary characterization, the possibility to obtain low-damage growth of a-Si:H and nc-Si:H thin films has been assessed. The trend of the crystallinity as a function of the electron temperature has also been presented, and its relationship with the low potential-drop allowed by this source at plasma-substrate interface has been discussed.

EN-ThP12 Relationship Between Interface Microstructures and Obtainable Photovoltaic Properties in ZnO/Cu₂O Heterojunction Solar Cells, Y. Nishi, S. Abe, T. Miyata, T. Minami, N. Ikenaga, O. Ueda, Kanazawa Institute of Technology, Japan

In this paper, we present our investigation into the relationship between the observable microstructure at heterojunction interfaces and the obtainable photovoltaic properties in ZnO/Cu₂O heterojunction solar cells fabricated with various structures on thermally oxidized Cu₂O sheets. Recently, we reported that high efficiencies of 2.19 and 4.12% as well as open circuit voltages of 0.5 and 0.72 V were obtained in heterojunction solar cells fabricated with an Al-doped ZnO (AZO)/Cu₂O or AZO/non-doped ZnO/Cu₂O structure, respectively: solar cells fabricated by depositing thin films on thermally oxidized Cu₂O sheets at room temperature using a pulsed laser deposition (PLD) method [1,2]. The improvement in obtained photovoltaic properties suggests that it is necessary to stabilize the surface of Cu₂O sheets as well as develop low-damage and low-temperature deposition techniques for forming and applying heterojunctions. In addition to improvements in the surface condition of Cu₂O sheets, the significant improvement of obtained photovoltaic properties exhibited in AZO/non-doped ZnO/Cu₂O heterojunction solar cells is attributable to enhanced potential barrier height and carrier lifetimes near the interface, resulting from the inserted buffer layer functioning as an n-type ZnO layer as well as an active layer in the n-p heterojunction. Cross-sectional views of ZnO/Cu₂O heterojunctions obtained by transmission electron microscopy revealed interface microstructures that differed significantly between high-efficiency and low-efficiency solar cells, fabricated with different deposition conditions, irrespective of the device structure used. For example, in AZO/non-doped ZnO/Cu₂O heterojunction solar cells fabricated with both the AZO and non-doped ZnO thin films prepared by PLD at the same deposition temperatures, either RT or 200°C, the solar cells formed at RT exhibited higher efficiency than those formed at 200°C. A smooth heterojunction was observed near both the interfaces within AZO/non-doped ZnO/Cu₂O heterojunction solar cells fabricated at RT; this contrasts with many dislocations observable near both of these interfaces of solar cells fabricated at 200°C, *i.e.*, between the non-doped ZnO layer and the Cu₂O and between the AZO and non-doped ZnO layers. Thus, the TEM observations of the heterojunction solar cells fabricated by forming both thin films at RT indicate that the higher efficiency results from an increase of carrier lifetimes, a consequence of suppressing carrier recombination and trapping near the interfaces of the heterojunctions.

[1] Y. Nishi et al., *Thin Solid Films*, 520 (2012) 3819.

[2] Y. Nishi et al., *J. Vac. Sci. Technol. A* 30 (2012) 04D103.

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