Nano-based Approaches for Photovoltaics

Moderator: Jason Baxter, Drexel University, USA

8:40am EH-MoM1 Thin Film Solar Cells from Colloidal Nanoparticle Dispersions, Eray Aydil, B. Chornomordik, N. Trejo, University of Minnesota

The global installed capacity to generate electricity using solar cells has doubled every 2.5 years since 1975, an exponential growth similar to the Moore’s law which states that the number of transistors on a computer chip doubles every 2 years. Maintaining this aggressive Moore-like growth requires sustainable, high-throughput low-cost production of thin film solar cells. Copper zinc tin sulfide (Cu2ZnSnS4 or CZTS), copper zinc tin cations. Finally, a demonstration of how the obtained results can help to engineer a more stable structure is presented.


The employment of solution based methods for the deposition of semiconductor materials for solar cells applications comes with promise of enabling large area applications at the same time of driving down costs. The optimization of thin film semiconductors such as CuZnSnS requires the understanding of the structure and chemical reactions taking place during deposition of thin films and post-deposition thermal treatments. In this respect, X-ray photoelectron spectroscopy (XPS) is uniquely suited for tracking down chemical reactions occurring at the surface and interface of nanometric layers. The chemical analysis and thermal stability for surface and interface reactions of binary chalcogenide semiconductors is presented. CuS, ZnS, and SnS thin films were deposited on top of CdS by the successive ionic layer absorption and reaction method (SILAR) in a glove-box attached to the XPS load-lock chamber for in-situ analyses. Step by step XPS analysis of the SILAR process reveals an incubation period that depends on temperature and ion concentration. Multilayer structure stability is discussed in terms of chemical reactivity and diffusion of cations. Finally, a demonstration of how the obtained results can help to engineer a more stable structures is presented.

10:40am EH-MoM6 Nanoscale Characterization of Defects and Interfaces in Thin Film Solar Cells, Mowafak Al-Jassim, NREL

Thin-film solar cells based on polycrystalline CdTe, CuIn(Ga)Se2 (CIGS), and Cu2ZnSnSe4 (CZTSe) have demonstrated high solar-to-electricity conversion efficiencies. Typically, polycrystallinity in thin-film solar cells is expected to exhibit poor performance compared to their single-crystalline counterparts, due to the existence of unavoidable structural defects such as dislocations and grain boundaries (GBs). It is surprising, therefore, that CdTe, CIGS, and CZTSe-based polycrystalline thin-film solar cells have achieved higher efficiencies than their single-crystalline counterparts. Here, we present our results on the study of the atomic structure and electronic properties of structural defects including stacking faults, twins, dislocations, and GBs in CdTe, CIGS, and CZTSe using a combination of aberration-corrected scanning transmission electron microscopy (STEM) and first-principles density-functional theory calculation. Polycrystalline CdTe thin films were grown by close-space sublimation, whereas CIGS and CZTSe thin films were deposited by co-evaporation. Atomic resolution scanning transmission electron microscopy (STEM) images were acquired with Nion UltraSTEM 100 and 200 microscopes. We found that intrinsic GBs in CdTe, CIGS, and CZTSe create deep levels mainly due to the anion-anion “wrong” bonding. However, these deep levels can be removed through extrinsic and/or intrinsic passivation. I addition to high resolution structural and chemical characterization, we will present data on the electronic and optoelectronic properties of defects obtained by a correlation approach that involves STEM, cryogenic cathodoluminescence defect spectroscopy and electron beam induced current imaging.

11:00am EH-MoM8 Charge Transport in PbS Quantum Dot Arrays for Photovoltaic Applications, Miquel B. Salmeron, Lawrence Berkeley Lab, USA

New forms of matter can be designed by combining nanoscale building blocks to create artificial solids with novel functionalities for device applications, such as field effect transistors, solar cells, photodetectors, and light emitting diodes. Artificial atoms or quantum dots (QDs) are ideal elements for this purpose since their electronic properties can be tuned over a wide range of size, shape, and composition, while charge transport through QD assemblies can be engineered by controlling the hopping barrier between neighboring dots. However, fabrication of the QDs comprised of hundreds to thousands of atoms is inevitably imperfect and defects and impurities are always present. The nature of the defect states is unknown and the microscopic (molecular) origins of their electronic properties are far from being understood. In this presentation we show, by means of nanoscale imaging, spectroscopy, and density functional theory (DFT), that charge transport takes place in PbS QD arrays following percolation pathways that are spatially different for electrons and holes, electrons via in-gap states (IGS) instead of conduction band states, and holes via valence band states. This novel and exotic transport phenomenon is explained by the measured electronic structure and energy level alignment of the individual QDs. In contrast with previous hypothesis that surface stoichiometry and ligands are relevant, we found that the IGS are induced by adsorbed oxygen molecules whose states hybridize with QD valence band states, thus enabling inter-particle coupling and electron transport. We demonstrate that chemical treatments can be used for surface impurity engineering to achieve tunable electronic structure and transport properties.

11:40am EH-MoM10 The Effect of n and p Delta Doping on InAs/GaAs Quantum Dot Solar Cell, W.J. Choi, HoSung Kim, S.H. Kim, J.D. Song, W.J. Choi, InAs/GaAs Quantum Dot Solar Cell, S.H. Kim, J.D. Song, Korea Institute of Science and Technology, Republic of Korea, J.H. Park, Korea University, Republic of Korea

The efficiency of single junction solar cells (SJSs) is limited by Shockley-Queisser limit and intermediate band solar cell (IBSC) concept has been introduced to bridge the efficiency limit of conventional SJSC. For IBSC model, low dimensional semiconductor structures such as quantum wells and quantum dots (QDs) have been applied to the SJSC. Especially, self-assembled InAs QDs have been frequently applied to GaAs/AlGaAs SJSs because QDs provide quantum confined states that lower the average band gap of the SJSs to absorb longer wavelength light beyond GaAs band edge of 870 nm. Theoretical studies of QDSCs have suggested a maximum efficiency of 45 % under 1 sun and 63 % under 1000X concentration. Contrary to their expectations,
actual QDSC devices suffer from photocurrent loss due to inhomogeneous distribution in QD sizes and high carrier confinement of QDs. In order to solve these problems, n delta doping techniques on QDs have been investigated. Here, we introduce the result of QDSCs with n and p delta doping on QDs.

For this study, two types of SC samples were grown on N-GaAs substrate and P-GaAs substrate respectively by molecular beam epitaxy. The undoped and delta-doped QDSCs with doping density of $1 \times 10^{12} \text{ cm}^{-2}$ were prepared and every SC samples has spacer layer with thickness of 20 nm between InAs QD layer and delta doping layer. SC samples grown on N-GaAs and P-GaAs substrate were delta doped with Si and Be respectively. The InAs QDs were grown by modified Stranki-Krastanov growth method. With this growth technique, the QD size and density can be controlled by using the repetition period of a cycle.

The efficiency of QDSCs with and without Si delta doping are 13.6 % and 11.4 % respectively. The enhancement of the efficiency of QDSCs with Si delta doping is due to the increase of $J_{sc}$. This increase of $J_{sc}$ is due to the n-delta doping and this enhances electron transitions in QDs and increase the carrier lifetime in QDs. The efficiency of QDSCs with and without Be delta doping are 8.45 % and 10.9 % respectively. Compare to the result of QDSCs grown on N-GaAs substrate, the efficiency of QDSCs with Be delta doping has been decreased. This could be attributed to the P delta doping. The Be delta doping induces suppression of the photocarrier generation in the radiative QDs because intentionally doped holes are strongly localized in the radiative QDs. We will present the result of the time-resolved photoluminescence of the QDSCs with Si and Be delta doping.
Meeting the world’s growing energy needs in a sustainable fashion is one of the most pressing problems of our time. The most abundant source of renewable energy is the sun, which can be converted directly to useful energy. Solar cells convert sunlight into electricity, and progress in developing more efficient solar cells is a major research focus. One area of active research is the use of colloidal quantum dots (QDs), which are nanoscale materials typically based on low-band-gap metal chalcogenides, have been widely explored for next generation solar absorbers due to their tunable band gap and high absorption coefficient. Colloidal quantum dot (CQD) solar cells made from lead sulfide (PbS) QDs have achieved a power efficiency of ~ 8%. In these devices, it is important to control the band gap as well as the band alignment of the QDs with the electrodes to efficiently inject electrons and holes into their respective electrodes. We will describe experimental and theoretical studies of the effects of interface engineering through surface ligand modification on the band gap and relative band positions in lead chalcogenide (PbSe, PbS, PbTe) QDs. Multilayer CQD solar cells were fabricated to investigate the effect on carrier collection of QD layers with different relative band positions. We will show that interface engineering can be applied to lead chalcogenide QDs in order to create a favorable band diagram and achieve enhanced photogenerated carrier collection in multilayer CQD devices.

Energy Harvesting & Storage
Room: Lehua - Session EH-TuM

Solar Cells
Moderator: Eray Aydil, University of Minnesota

08:45am EH-TuM3 Understanding and Improving Solar Energy Conversion through Interface Engineering. Stacey Bent, Stanford University, USA

Today CdS/CdTe heterojunction is an important photovoltaic system for conversion of solar energy. Due to the simple techniques used for thin films deposition, it has been brought from laboratory to industrial scale. Although the thin films are deposited by using techniques such as sputtering and CSS, the back contact layers are a challenge in both: the formation of an ohmic contact and that endures a long time. There are several prospects for back contacts using Mo as can be seen in [1]. The solar cell with Cu/Mo as a back contact deposited by using rf-sputtering is reported in [2]. There are few researches that studied how Mo film can be protected against oxidation without adding series resistance. The bilayer Mo/ITO has been used in microelectronics devices [3].

In this work, the CdS/CdTe solar cells that uses Cu/Mo as back contact is investigated. It is shown that the formation of MoOx at surface of Mo thin film influences the series resistance. The oxide is formed when the solar cell is used at outdoor conditions without any encapsulation. Here some indoor experiments were made. First, we show how the Mo/Glass film is oxidized when it is annealed at 400 °C in air. Second, how the Mo is degraded at same conditions when it is used on CdTe/CdS cell and annealed at same condition. Finally, how ITO works when it is deposited over Mo as the back cell. Preliminary results indicates that the ITO avoids the formation of MoOx and mechanical scratching , preserves its electrical properties and the solar cell shows good stability after an annealing at 400 °C.

09:20am EH-TuM5 Understanding Carrier Dynamics in Cu2ZnSn(S,Se)4 Using Time-Resolved Terahertz Spectroscopy. G.W. Guglietta, Drexel University, USA, K. Roy Choudhury, J.V. Caspar, DuPont Central Research and Development, USA, Jason Baxter, Drexel University, USA

We have used time-resolved terahertz spectroscopy (TRTS) to measure lifetimes and determine recombination mechanisms in Cu2ZnSn(S,Se)4 (CZTSSe) thin films fabricated from nanocrystal inks. TRTS probes photoconductivity on femtosecond to nanosecond time scales that are relevant for recombination in thin film photovoltaics. Terahertz frequencies (0.2-2.5 THz) correspond to typical scattering rates in semiconductors, enabling the determination of carrier density and mobility. Ultrafast time resolution permits tracking the evolution of carrier density to determine recombination mechanisms. By manipulating the photoexcitation wavelength and fluence, we can tailor the generation profile of photoexcited carriers to distinguish between surface, Shockley-Read-Hall (SRH), and Auger recombination mechanisms and determine rate constants. TRTS experiments and modeling were used to understand the role of recombination mechanisms and their contribution to CZTSSe photovoltaic performance. TRTS photoconductivity shows an instrument-limited onset within 1 ps of an ultrafast pump pulse, followed by a slow decay over nanoseconds. Photoconductivity decay kinetics were fit with a bi-exponential model with two time constants and a weight fraction. Measurements were performed at LANNIBO CINVESTAV-Mérida, under support from projects FOMIX-Yucatán 2008-108160, CONACYT-LAB-2009-01 No. 129913 and CB2012-178947.

References

10:05am EH-TuM6 The CdS/CdTe Solar Cell with the Back Contact Protected by ITO/Mo, Juan Peña, V. Rejoń, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Mexico, M. Riech, Universidad Autónoma de Yucatán, Mexico. N. Hernández-Rodríguez, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, Mexico

Today CdS/CdTe heterojunction is an important photovoltaic system for conversion of solar energy. Due to the simple techniques used for thin films deposition, it has been brought from laboratory to industrial scale. Although the thin films are deposited by using techniques such as sputtering and CSS, the back contact layers are a challenge in both: the formation of an ohmic contact and that endures a long time. There are several prospects for back contacts using Mo as can be seen in [1]. The solar cell with Cu/Mo as a back contact deposited by using rf-sputtering is reported in [2]. There are few researches that studied how Mo film can be protected against oxidation without adding series resistance. The bilayer Mo/ITO has been used in microelectronics devices [3]. In this work, the CdS/CdTe solar cells that uses Cu/Mo as back contact is investigated. It is shown that the formation of MoOx at surface of Mo thin film influences the series resistance. The oxide is formed when the solar cell is used at outdoor conditions without any encapsulation. Here some indoor experiments were made. First, we show how the Mo/Glass film is oxidized when it is annealed at 400 °C in air. Second, how the Mo is degraded at same conditions when it is used on CdTe/CdS cell and annealed at same condition.

The CdTe film was grown by conventional CVD technique. The cells were activated by using CHClF2-argon-oxygen gases. DRX spectra and HR-SEM were made for Mo/Glass and ITO/Mo/CdTe structure before and after annealing at 400 °C in air.

Acknowledgement
This work has been supported by CONACyT-México under contract FORDECyT-116157, FOMIX-169739 and FOMIX-172298, CeMIE-Sol PY-207450/25. Measurements were performed at LANNIBO CINVESTAV-Mérida, under support from projects FOMIX-Yucatán 2008-108160, CONACYT-LAB-2009-01 No. 129913 and CB2012-178947.

References

10:20am EH-TuM8 Study of Energy Level Alignment at Electrode Interfaces in Organic Solar Cells. Takeaki Sakurai, S. Wang, T. Miyazawa, H. Xiu, W. Fu, K. Akimoto, University of Tsukuba, Japan

Control of electrical properties at organic semiconductor/metal electrode interfaces is one of the significant issues for improving performances of the organic solar cells since it has an influence on carrier extraction and exciton quenching. In small molecule based organic solar cells, bathocuprine (BCP) is used well as a buffer layer between C60 and metal cathode to improve the device efficiency. Lifetime and the stability of the device with BCP buffer layer, however, are not good for the practical application. To obtain the strategies for the development of the effective buffer layer, we have investigated the electronic structures at the interfaces between C60 and a large variety of organic semiconductors by means of synchrotron based in-situ ultraviolet photoelectron spectroscopy. The C60/buffer/Ag heterostructures were formed by depositing buffer materials on Ag and subsequently depositing C60 onto buffer/Ag stack layer in a step-by-step way in a vacuum deposition chamber. A series of perylene derivatives (PTCDI, PTCDI and PTCDI), TNQ derivatives (TNQ and F4TCNQ) and pyrindine based acceptor molecules (BCP, TPBi and TAZ) were applied as buffer layers. For all buffer/Ag stack structures, the LUMO level of buffer layers almost accords with Fermi level of Ag, that is, electron is easily transferred from the Ag electrode to the buffer layers due to the disappearance of the electron injection barrier. In contrast, the electron injection barrier height between LUMO of C60 and LUMO of buffer materials correlates with the work function of the buffer/Ag stack structures.
We conclude that to select a buffer/Ag heterostructure with low work function is important in order to maintain good electric contact near Ag cathode. The detailed physical mechanism about the energy level alignment will be discussed using charge transfer model.

11:00am  **EH-TuM10  n-type Thin Film WSe\textsubscript{2} for use in Homojunction WSe\textsubscript{2} Solar Cells**, A. Sarkar, Natale Ianno, R.J. Soukup, University of Nebraska-Lincoln

Previously we have shown that as-grown p-type thin film WSe\textsubscript{2} is an excellent candidate for an earth abundant photovoltaic absorber. The vast majority of thin solar cells are heterojunction devices with a wide band gap n-type window layer. Many of the device issues are centered on the heterojunction interface, making a homojunction more desirable. The problem here is growing n-type material in thin film systems. In this work we present the structural, optical, and electrical properties of n-type thin film WSe\textsubscript{2} grown via the selenization of sputter deposited copper doped tungsten films. We will show that highly textured films with an optical band gap in range of 1.45 eV, and absorption coefficients greater than 10\textsuperscript{5}/cm across the visible spectrum can be easily achieved. In addition we will present Hall Effect and carrier density measurements as a measure of film quality. We employ these results to numerically simulate homojunction solar cells based on this material, where we will show efficiencies greater than 20% are possible.


A new research thrust to obtaining high efficiency photovoltaic systems is spectrum splitting, where the input solar radiation is physically separated via input optics and channeled to a planar array of individual cells, each with a band gap tuned to absorb a specific band width of radiation. This approach allows for simpler device fabrication and a wider breadth of band gaps than the common multi-junction design, in exchange for a complex optics structure to separate the incoming light. Both these approaches require high efficiency cells over a broad range of band gaps. Currently this is met by III-V alloy single crystal cells and while significant advances have been made in reducing the fabrication cost, recent best estimates place their cost at 1-5x single crystal silicon cells. In addition many of these materials contain indium, whose supply may be limited.

In order for the multi-junction and split spectrum designs to fully realize their potential, it is necessary to explore other classes of semiconducting materials with tunable band gap, better crustal abundance and lower production costs. The Sm\textsubscript{2-x}Ce\textsubscript{x}S\textsubscript{3} alloy system with its potentially broad band gap range (0.8-1.9 eV), as grown p-type majority carrier, potentially excellent optoelectronic properties in polycrystalline form and abundance is an excellent candidate. We will present preliminary data on the growth, optical and electrical properties of thin film Sm\textsubscript{2}S\textsubscript{3}, and Ce\textsubscript{2}S\textsubscript{3} as an initial study of the alloy formation.
Energy Harvesting & Storage
Room: Mauka - Session EH-TuP

Energy Harvesting & Storage Poster Session

EH-TuP4 Synthesis and Hydrogen Properties of Beryllium Intermetallic Compound, Jae-Hwan Kim, Japan Atomic Energy Agency, Japan, H. Furihata, University of the Ryukyus, Japan, M. Nakamichi, Japan Atomic Energy Agency

Beryllium intermetallic compounds have shown a variety of excellent properties, such as neutron multiplier, refractory function, hydrogen storage, superconductivity and so on. Be₂M compounds (M=Ti, V and Zr) have been investigated as neutron multiplier in fields of fusion reactor while Be₁₂M compounds have been focused on refractory materials. In addition, Be₂M have been known as a Laves phase which is characterized by an AB₂ type compound performing higher H₂ gas storage potential. Although great interest on hydrogen properties of Be₂M owing to its lower density has been aroused from viewpoints of reactivity with H₂O, trap site of hydrogen and amount of H₂ gas in this compound, few studies on the Be₂M found and its data base is still unsatisfactory.

In this study, we report on preliminary synthesis of Be₂Ti compound and its properties, such as hydrogen generation rate with H₂O and hydrogen storage. Additionally, first principles calculation of hydrogen trap site in this compound was carried out in order to compare to empirical data. X-ray diffraction profiles and electron probe micro-analysis results clarify that the preliminary synthesis of Be₂Ti was successful by homogenization treatment and plasma sintering. Hydrogen generation rate of the Be₂Ti by a reaction with 1 % H₂O increased as test temperature increased. High temperature exposure with H₂O leads to formation of TiO₂ on the surface. In addition, hydrogen storage result of Be₂Ti evaluated by pressure-concentration-temperature curve depicts that Be₂Ti indicated H₂ gas storage concentration with 1.6 w.t. % at 323 K when the H₂ pressure increases up to 10 MPa. According to the first principle calculation, there were two hydrogen trap sites, tetrahedron and center of triangle with solids energies of -0.52 and -0.05 eV, respectively, indicating maximum trap site with 5.4 w.t. %.

EH-TuP5 Characterization of Real Cyclic Performance of Air Electrode for Li-Air Batteries. DaeHo Yoon, Y.J. Park, Kyonggi University, Republic of Korea

In this study, we characterized the cyclic performance of an air electrode employing a carbon nanotube (CNT)/Co₃O₄-nanocomposite. The lithium anode and electrolyte were replaced every 50 cycles in order to exclude the effect of a corrupted anode and electrolyte and to determine the “real” cyclic performance of the electrode. The overpotential of the cells increased during the first 50 cycles; however, it almost vanished when the lithium anode and electrolyte were replaced. This result indicates that the increased overpotential of the cells during cycling is highly attributed to the corrupted lithium anode and electrolyte [1, 2]. The cycle life of the cell also significantly increased upon replacement of the lithium anode and electrolyte. This confirms that air electrodes have the ability to maintain their designated capacity (such as 1000 mAh·g⁻¹) for much longer cycles if the lithium anode and electrolyte can be made more stable. A polydopamine-coated electrode and a LiF-containing electrolyte were introduced and characterized in order to obtain enhanced cyclic performance of the air electrode.

References
[2] Jun Lu, Yu Le, Nature Communications DOI:10.1038/ncomms3383

EH-TuP6 Nano-Sized Li[Li0.2Ni0.16Mn0.56Co0.08]O2/Super P Composite for Improving Electrochemistry Performance. S.B. Lim, Kyonggi University, YongJoon Park, Kyonggi University, Republic of Korea

Since the commercialization of lithium ion battery, development of cathode materials with high capacity has been one of the important factors for enhancing the performance of that. Lithium rich compounds are promising cathode materials due to their high capacity for satisfying demand of high-capacity batteries. However, they have several disadvantages to overcome for commercialization such as poor rate capability, low cyclic performance, and low stability. In this study, we prepared nano-sized Li[Li0.2Ni0.16Mn0.56Co0.08]O2/carbon composite for enhanced electrochemical performance such as rate capability. A general method to improve the surface electronic conductivity and enhance the rate capability of cathode is carbon coating. The carbon coating by in-situ carbonization from organic precursors has been successfully applied to LiFePO₄. However, it is difficult to apply to Li-rich compounds because they will lose oxygen during carbonization. That is why we introduced composite between cathode and carbon, instead of carbon coating. In this work, super P, a commercial carbon, was used with nano-sized Li[Li0.2Ni0.16Mn0.56Co0.08]O2/Super P, coarse powders were synthesized by combustion method using surfactants (HPC and Gelatin) to disperse the granule particles [1-3]. The polydopamine pre-coating layer was used as a binding agent between cathode powder and super P [4-8]. Nano-sized Li[Li0.2Ni0.16Mn0.56Co0.08]O2/Super P composite is expected to exhibit improved rate capability because of dispersed nano-sized lithium rich particles and good electronic conductivity attributed to Super P.

EH-TuP8 Fabrication of Structured Organic Solar Cell with Patterned ITO Electrode and Study of Their Effect on Power Conversion Efficiency. Jin-Hyo Boo, J.S. Lee, Sungkyunkwan University, Korea

In organic photovoltaics (OPVs), there is a competition between the reduction of absorber thickness and the improvement of the probability of carrier collection. To overcome the competition a highly structured interface is highly desirable. However, a solution-based soft-lithography processing resulted in non-uniform structured surfaces. In this report, we proposed and demonstrated a silica-templated soft-lithographical approach for structuring well-defined and controllable ITO layer for enhancing power conversion efficiency (PCE). Also, we focused on the morphological effects of the patterned ITO on optical properties and PCE.

The brief experimental scheme is as follow. First, close-packed PS nanospheres were formed on a cleaned ITO glass substrate by using gas-liquid-solid interfacial self-assembly method and drying for 3 days in vacuum desiccator. After that, PS covered ITO glass was etched at 65°C with TIN etching solution. Finally, PEDOT:PSS, P3HT:PCBM, and Al electrode were gradually deposited.

The morphology, optical, electric, and cell properties are investigated by FE-SEM, AFM, UV-VIS spectrophotometer, Haze measurement, and solar simulator.

EH-TuP9 Supercapacitive Properties of 2D-arrayed Inverse-Opal Nanostructure of Manganese Oxide. Ilhwan Ryu, D. Park, G. Kim, S. Yun, Kookmin University, Republic of Korea

Supercapacitor has attracted growing attention as an important energy conversion and storage device which basically consists of current collector, electrolyte and active materials. Manganese oxide (MnO₂) is one of the most promising active materials due to its environmentally friendly characteristic and low price. Fabrication of nanostructured active materials has also been widely studied since it can provide large surface area and short diffusion path for ions and electrons, and hence improve the capacitive properties of the supercapacitors. In this work, we fabricated well-ordered MnO₂ inverse-opal nanostructures using two-dimensionally arrayed polystyrene nanospheres. We also investigated their optical, morphological and electrochemical properties, and compared them with the properties of the device based on the planar MnO₂ films.

EH-TuP10 Inorganic-organic Core-Shell Nanowire Solar Cells with Excellent Light-Trapping Properties. Keisuke Sato, Tokyo Denki University, Japan, M. Dutta, N. Fukata, National Institute for Materials Science, Japan

Development of solar cells using one-dimensional architecture, such as semiconductor nanowires (NWs), have been proceeding rapidly in recent years. The main advantage of such NWs-based solar cells is that they cause greater light absorption (minimal reflectivity) due to incident light-trapping within the NW arrays. This phenomenon is most glaringly apparent in silicon nanowires (SiNWs)-based solar cells, leading to higher absorbance per unit thickness than achieved by commercial crystalline Si solar cells. Thus, the introduction of the SiNW arrays with high light-trapping properties enable lower-cost cell production due to the massive reduction of the consumption of Si materials needed for cell fabrication. We have developed inorganic-organic core-shell NW solar cells in which the vertically-aligned SiNWs were surrounded by organic poly(3,4-
ethylendioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) layer in order to further facilitate the cell fabrication. We report herein on the cell performances of Si-PEDOT:PSS core-shell NW solar cells with excellent light-trapping properties. To investigate the light-trapping capability, the lengths of the core-shell NWs were varied within the range from 2 to 8 μm. In the core-shell NWs with shorter length of 2 μm, the reflectance were suppressed to below 8%, which is extremely lower than the crystalline Si with value of 31%, over a wide spectrum range between 300 and 1000 nm. This suppression in reflectance was made effective for longer NW length, resulting in a reflectance of below 4.6% for the core-shell NWs with longer length of 8 μm. These results demonstrate that the longer core-shell NW arrays can extend the broadband anti-reflection effect due to enhanced light-trapping in NW arrays. However, the cell performances of such core-shell NW solar cells closely were intimately related to the NW length-dependent carrier transport efficiency. The light-trapping effects of NW solar cells with shorter length of 2 μm exhibited the best cell performance with a power conversion efficiency (PCE) of approximately 7%, exceeding those with longer length of 8 μm (PCE of 3.7%). The depression of cell performance with the increase in the NW length was caused by inefficient carrier collection at electrodes due to the enhancement of the carrier recombination, because the transportation distances to electrodes were increased with NW length. Therefore, we suggest that it is important to simultaneously tune the NW length and light-trapping properties to be able to fabricate efficient inorganic–organic core-shell NW solar cells.


In photovoltaic solar cell, CdS thin films are mostly used buffer layer due to their wide direct bandgap (~2.4 eV). The CdS buffer layers which form a p-n junction with absorber layer are deposited by using a variety of deposition methods such as chemical bath deposition (CBD), spray pyrolysis, vacuum-evaporation and sputtering. Among these techniques, chemical bath deposition is widely used method due to its advantages such as easy and inexpensive process. However, CBD technique also has disadvantages such as damage of substrates including production of toxic waste containing Cd and ammonia and difficulty in application to mass production scale. In addition, CBD method should be done in liquid phase, so that it can oxidize the absorber layer.

To overcome these disadvantages of CBD method and to apply for large scale deposition, sputtering of Zn(O,S) thin films was proposed. Sputtering method of Zn(O,S) films can reduce the liquid wastes and save the deposition time for fast deposition. It enables all processes for solar cells to be carried out by vacuum processes without exposure to air. In addition, Zn(O,S) thin films can replace the CdS which contains a toxic Cd. Generally, Zn(O,S) thin films can be deposited by sputtering with pure ZnS target by adding oxygen or by co-sputtering using ZnO and ZnS targets. ZnS itself has very high band gap about 3.6 eV, so that oxygen should be added to control the band gap. Currently, their electrical and optical properties of these Zn(O,S) films are under investigation. In this study, Zn(O,S) thin films are deposited on Cu(In,Ga)Se₂ layer and glass substrate by RF sputtering in an O₂/Ar atmosphere using pure ZnS target. The CIS solar cells having the Zn(O,S) thin films on Cu(In,Ga)Se₂ layer were fabricated. The solar cells' current density–voltage (J-V) characteristics were investigated both in the dark and under AM1.5G illumination by a solar simulator (Keithley 69911). Keywords: CuInSe₂, Binary compound, Solar cell, Wet process, PhotoluminescenceAcknowledgment This work was supported by the New & Renewable Energy Core Technology Program of the Korea Institute of Energy Technology Evaluation (No. 2013300011330) and the Human Resource Development Program (No. 20140410100500) Planning (KETEP), granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea.

**Eh-TuP13 In-situ Investigation of phase Evolution during Cu₂ZnSnSe₄ Thin Film Photovoltaic Absorber Formation from Various Stacked Cu-Zn-Sn Precursors, Hyeonwook Park, J. Han, W.K. Kim, Yeungnam University, Republic of Korea.**

For several decades, chalcopyrite Cu(InGa)Se₂ (CIGS) thin films were considered as a potential candidate for use as light absorbers in high-efficiency thin film photovoltaic cells. Recently, a cell efficiency of 20.9% (Solar Frontier, 2014), which is a little bit higher than multi-crystalline Si cells (20.4%), has been reported. Over the last decade, great attention has been moved to kesterite CuZnSn(S,Se)₄ (CZTSSe) as a promising low-cost alternative to chalcopyrite CIGS. In this paper, temperature-dependent x-ray diffraction analysis is carried out to investigate the phase transformation pathway of kesterite CuZnSnSe₄ (CZTSSe) thin film photovoltaic absorber formation by selenization of various stacked precursor structures including (Cu+Sn)/Zn and (Cu+Zn)/Sn were systematically investigated using in-situ high temperature X-ray diffraction system, consisting of a PANalytical X’pert Pro MPD diffractometer and an Anton Paar HTK 1200 N furnace. A custom-designed graphite dome was utilized in order to create Se vapor at the elevated temperatures and minimize the loss of vaporized Se. Furthermore, CZTSSe films formed by selenization of stacked Cu-Zn-Sn/Se precursors were characterized by X-ray diffraction and raman spectroscopy. The results revealed that the formation temperature of CZTSe and detailed phase evolution would be affected by stacked structure of Cu-Zn-Sn. Furthermore, precursor structure with co-sputtered Cu and Sn (e.g., (Cu+Sn)/Zn and Zn/(Cu+Sn)) could reduce Sn loss effectively during the formation of CZTSe than that with single-layered Sn (e.g., (Cu+Zn)/Sn and Sn/(Cu+Zn)).
incident photon-to-electron conversion efficiency (IPCE), and intensity-modulated photocurrent spectroscopy (IMPS) / intensity-modulated photo voltage spectroscopy (IMVS), DSSC with this material shows a high-energy conversion efficiency of 8.2% at 100 mWcm⁻². This is one of highest values for N719-based, solid-state, dye-sensitized solar cells.

**EH-TuP16 Effect of MoN Diffusion Barrier on High Temperature Selenization of Cu(In,Ga)

Min-Su Kwon, H.-G. Kim, S.-H. Kim, C.-W. Jeon, Yeungnam University, Republic of Korea

In commercial manufacturing of CIGS photovoltaic module, the absorber films are usually produced by sputtering and selenization/sulfurization process. During high temperature selenization above 450°C, the surface of Mo back contact is easily transformed to MoSe₂, which is beneficial for ohmic contact formation in Mo/CIGS interface.[1] Although MoSe₂ has a high resistance, because it is a semiconductor of having bandgap energy of 1.35–1.41 eV, the thin layer of 100nm or less does not adversely affect the characteristics of solar cell.[2] However, since MoSe₂ may provide a current blocking capability when thicker than 200nm, it is necessary to control the thickness of the MoSe₂. In this study, Mo/MoxN/Mo multi-layer back contact was selenized to evaluate capability of diffusion barrier of MoxN layer to prevent the excessive MoSe₂ formation. The CIGS absorber films were obtained by solid state selenization, where a sputtered CuInGa alloy film on Mo/MoxN/Mo/glass was subsequently selenized at 460~560 °C for 10 minutes by using Se vapor. Behavior of generated MoSe₂ was analyzed by using XRD, SEM. The conducting compound of MoxN as a diffusion barrier against Se was deposited by a reactive sputtering. The thickness and N content of MoxN was found to be linearly proportional to N₂ gas flow rate, which suggests that MoxN could be easily adjusted by a simple modification of Mo formation process. As a result of selenization, because of the formation of MoSe₂, thickness of Mo mono-layer precursor was abruptly increased. But the thickness of multi-layered back contact with MoxN was not changed significantly. Therefore, as a diffusion barrier, MoxN was confirmed to be excellent diffusion barrier that is suited for a high temperature selenization process. The effect of MoxN layer on solar cell performance will be discussed. Acknowledgements This research was financially supported by the Ministry of Knowledge Economy(KME), Korea Institute for Advancement of Technology(KIAT) and Dae-Gyeong Leading Industry Office through the Leading Industry Development for Economic Region). References [1] P.J. Rostan*, J.Mattheis, G.Bilger, U. Rau, J.H. Werner, Thin Solid Films Volume 480-481, Pages 67-70(2005). [2] SeJin Ahn, Ki hyun Kim, Jae Ho Yun, and Kyung Hoon Yoon, Journal of Applied Physics 105, 113533(2009)

**EH-TuP17 Nano-patterned Pt Counter electrode Enhancing Light harvesting for Dye-Sensitized Solar Cells, Won Seok Chi, D.J. Kim, J.P. Jung, J.H. Kim, Yonsei University, Korea

Nano-patterning is one of the most simple and effective techniques for efficiently light trapping to boost the energy conversion efficiency. By imprinting with poly(dimethyl siloxane) (PDMS) nanostamp cross-rotate two steps onto thin layered commercial TiO₂ paste, a mesh-shaped (200 nm × 200nm) TiO₂ scaffold electrode with a large area was fabricated. Platinum (Pt) nanoparticles deposited onto TiO₂ pattern by diverse method such as sputtering, thermal deposition and UV-radiation deposition. The Pt nanoparticles distribution as mesh-shaped structure onto counter electrode was characterized by a field emission scanning electron microscope (FE-SEM) and an atomic force microscope (AFM). Moreover, the light trapping ability was measured reflectance by comparison of mesh-shaped patterned and non-patterned counter electrode as a function of angle. For the four cases : 1) patterned Pt counter electrode by sputtering, 2) non-patterned Pt counter electrode by sputtering, 3) non-patterned Pt counter electrode by thermal deposition and 4) patterned counter electrode by UV-radiation deposition were fabricated for all-solid-state dye-sensitized solar cells (ssDSSCs). Among them, patterned Pt counter electrode by sputtering assembled solar cell showed highest solar energy conversion efficiency up to 7.0%. This remarkable result, observed for N719 dye based DSSC, was due to enhanced light harvesting and superior surface area confirmed by incident photon-to current efficiency (IPCE), electrochemical impedance spectroscopy (EIS), and cyclic voltammetry (CV) measurements. More importantly, we believe this approach is universally applicable to a variety of electrochemical cells requiring Pt catalysts such as fuel cells and catalytic chemical reactors. Furthermore, this process could include nano- and micro-sized patterns and can be extended to metal nanoparticles other than Pt.
Energy Harvesting & Storage
Room: Lehua - Session EH-TuE

Batteries, Capacitors & Storage Materials
Moderator: Stacey Bent, Stanford University, USA

5-40pm EH-TuE1 Electrochemical Deposition of Organic-inorganic Composites for Supercapacitors, M. Bai, Xiaoxia Liu, Northeastern University, China

Electrochemical Deposition of Organic-inorganic Composites for Supercapacitors
Ming-Hua Bai, Xiaoxia Liu*
Department of Chemistry, Northeastern University, Shenyang, 110819, China

Electrochemical capacitors (supercapacitors) are widely recognized as an important class of energy storage devices. Development of high performance supercapacitors is highly desirable to meet the increasing demand for energy storage devices. Conducting polymers, including polyaniline (PANI) and polypyrrole (PPy) have promising applications in a variety of technologic fields, including supercapacitor. One-dimensional (1D) growth control of conducting polymer, directing to polymer nanofibers, has aroused great interest because an ordered arrangement of the polymer chains favours higher conductivity and better performance in charge storage. The growth of nanofibers is known to be intrinsic to PANI, however heterogeneous nucleation on the initially-formed PANI nanofibers would result in irregularly-shaped PANI particles. The suppression of this overgrowth on the surface active sites of initially-formed PANI nanofibers has been achieved by some chemical polymerization methods, including aqueous/organic interfacial polymerization, rapidly-mixed reactions, which led to the formation of nanofibrous PANI. However, only nonfibrous, granular powder PPy can be yielded by these methods since fibillar structure is not intrinsic for PPy and so it is very hard for PPy to grow one dimensionally. Electrochemical deposition is very attractive due to the ability to anchor the product onto substrate materials in the desired quantity, shape and size in one single step, enabling the final application to be performed easier.

In this work, we will present the one-dimensional growth of conducting polymer through electrochemical co-deposition with inorganic oxide. The local environment at the electrode surface for polymerization was performed easier.

We gratefully acknowledge financial supports from National Natural Science Foundation of China (project number: 21273029) and Research Foundation for Doctoral Program of Higher Education of China (project number: 2012042110024).

Acknowledgements

References

7:40pm EH-TuE7 Water as Promoter and Catalyst in Di-Oxygen Reactions at Aqueous and Organic Electrified Interfaces, Nenad Markovic, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

Understanding the role of water in di-oxygen electrochemistry at atomic and molecular levels is the key to driving technological innovations that are urgently needed to deliver reliable, affordable and environmentally friendly energy [1-4]. Surprisingly, all previous studies have treated the water molecule as reactants needed to satisfy the stoichiometry of the reaction, rather than as vital hydrogen-donor molecules that can promote the rates of transformation of oxygen intermediates to final products. It is the impact of water on di-oxygen electrochemistry that constitutes the focus of our paper. First, we introduce a universal model that is capable of rationalizing, and ultimately understanding, electrocatalysis of the oxygen reaction in aqueous media, as well as in Li2O2 electrochemistry in organic environments. The model is based on the formation of HOx-+ H2O (alkaline) and LiO2-xH2O (organic solvents) complexes that place water in a configurationally favorable position for proton transfer to O2 and HO2 intermediates that are formed on neighboring active sites. We propose that monometallic electrodes modified by omnipresent oxygenated spectators such as OHad and LiO2 are, in fact, bifunctional catalysts capable of facilitating different parts of the overall multi-electron process: providing adsorption sites for the formation of complexes as well as bare metal sites to facilitate the electron transfer to O2, HO2 and HO2.

Moreover, we demonstrate that water plays a dual role in Li2O2 electrochemistry, acting simultaneously as a promoter in the production of Li2O2 and also as a catalyst, regenerating itself through a sequence of steps that include the recombination of H+ and OH- back to water. Water acting as a catalyst has not, to the best of our knowledge, previously been reported for any electrochemical reaction.

References:

8:20pm EH-TuE9 Electrochemical Reduction of CO2 as a Way to Store Energy from Intermittent Sources, Paul Kenis, University of Illinois at Urbana-Champaign

The desire to increase the utilization of sustainable energy sources such as solar and wind is hampered by their intermittent nature. Large scale energy storage capacity is needed to maximize utilization of these sources,
specifically to avoid large amounts of renewable energy being wasted when their supply exceeds demand.

Over the last years we have studied the electrochemical reduction of \( \text{CO}_2 \) to various value-added chemicals such as carbon monoxide (CO), formic acid, and methane. When coupled to renewable energy sources such as wind and solar, this process can produce carbon-neutral fuels or commodity chemicals, possibly providing a method for storage of otherwise wasted excess energy from intermittent renewable sources [1].

For this process to become economically feasible, more active and stable catalysts as well as better electrodes are necessary such that \( \text{CO}_2 \) electrolyzers can be operated at sufficient conversion (current density >250 mA/cm\(^2\)), reasonable energetic efficiency (>60%), and sufficient product selectivity (Faradaic efficiency >90%). For CO production, a key reactant in the Fischer-Tropsch process, the best performance reported to date is current densities on the order of 90 mA/cm\(^2\) and energy efficiencies up to 45%, when operating at ambient conditions [2]. This presentation will focus on new catalysts systems for efficient conversion of \( \text{CO}_2 \) to CO: (i) Ag nanoparticles supported on TiO\(_2\) [3]; (ii) Au nanoparticles supported on multiwall nanotubes; and (iii) metal-free N-doped carbons. These catalysts have been characterized in a 3-electrode cell and in an electrolyzer. Current densities of between 100 and 250 mA/cm\(^2\) as well as energy efficiencies of up to 70% were obtained. The electrodes in all these cases are prepared using automated airbrushing [2], which reduced catalyst loadings to 0.75 mg/cm\(^2\) for Ag and 0.17 mg/cm\(^2\) for Au. These performance levels, together with the lower cost due to low precious metal loading (due to the use of catalyst supports), or even the elimination of precious metals altogether (N-doped carbons), brings electrochemical reduction of \( \text{CO}_2 \) to CO closer to economic feasibility.

We also performed an economic / life-cycle analysis of this process, to determine whether this technology can become, economically viable for large scale application in the storage of energy from renewable sources, and/or in the reduction of greenhouse gas emissions.

References
Hindering Effect of Surface Point-Defects for Photoreactivity on TiO\textsubscript{2}(110). Igor Lyubinetsky, Pacific Northwest National Laboratory

While surface point-defects are expected to act as charge trapping and/or recombination centers known in photoinduced processes, their direct impact of surface defects on photoreactivity is not well explored. We present the first observation of a suppressing effect of oxygen vacancy (V\textsubscript{O}) on photoreactivity of TiO\textsubscript{2}(110). Direct scanning tunneling microscopy imaging reveals a pronounced site-selectivity in the hole-mediated photooxidation of trimethyl acetate (TMA) on TiO\textsubscript{2}(110) upon ultra-violet light irradiation, wherein the reaction readily occurs at regular Ti sites but is completely inhibited at V\textsubscript{O} defects. Utilizing electron energy loss spectroscopy and density functional theory, we show that the lack of reactivity of TMA groups adsorbed at V\textsubscript{O} sites cannot be attributed to either a less active adsorption configuration or electron transfer from the V\textsubscript{O} defect. Instead, we propose that the excess unpaired electrons associated with the V\textsubscript{O} promptly recombine with photoexcited holes approaching the surface, effectively screening the TMA species at V\textsubscript{O} site. We also show that this screening effect is spatially short-ranged, being predominantly localized at the V\textsubscript{O} and only mildly affecting TiA's at adjacent Ti sites. The direct impact of O vacancies on TMA photoreactivity over TiO\textsubscript{2}(110) is expected to have similar implications for other hole-mediated (e.g., photooxidation) reactions in which adsorption at or near electronic point-defects is possible. Furthermore, the localized influence of these defects on hole-mediated chemistry offers opportunities for additional study of site-selective photocatalysis on TiO\textsubscript{2}.


* In collaboration with Z.-T. Wang and M.A. Henderson, PNNL and N.A. Deskins, Worcester Polytechnic Institute. We acknowledge support from the US DOE BES, Division of Chemical Sciences, Geosciences & Biosciences. A portion of this research was funded by the Chemical Imaging Initiative LDRD at PNNL.

Atomic Structure and Intrinsic Electronic States of the In\textsubscript{2}O\textsubscript{3}(111) surface. HolgerEisete Eisete, R. Zielinski, A. Lenz, Technische Universität Berlin, Germany, Z. Galazka, Leibniz Institute for Crystal Growth, Germany, M. Dähne, Technische Universität Berlin, Germany

Indium oxide as transparent semiconductor is one of the most promising materials for contact layers in photovoltaic applications. Nevertheless, due to the delicate fabrication process for single crystals only a few intrinsic properties are known about In\textsubscript{2}O\textsubscript{3} yet. Especially the storage under air conditions may influence the surface properties. Hence it is hard to decide, which properties are intrinsic and which ones are influenced by physisorbed and/or chemisorbed atoms and molecules from the ambient air.

In this contribution for the first time we studied high quality single crystals at their freshly UHV-cleaved (111) surfaces by scanning tunneling microscopy (STM) and spectroscopy (STS). From these investigations we achieve knowledge about the atomic configuration at the surface. This configuration fits well with recent density functional theory calculations, and indicate a local charge enhancement within the surface unit cell. Furthermore, STS reveals intrinsic electronic surface states within the fundamental band gap. The Fermi level is also energetically located within the fundamental bulk band gap, which leads to the assumption that previously reported electron accumulation at this surface is not an intrinsic property, but related to extrinsic effects, such as e.g., non-stoichiometric material reorganization. After oxidation of the In\textsubscript{2}O\textsubscript{3}(111) surfaces outside the UHV their structural as well as their electronic properties look quite different: astonishingly both show much more metallic behavoiur as the freshly cleaved ones kept under UHV-conditions. The processes leading to such an behaviour are still under discussions, but the data fits much better to previous observations.

Nanoporous gold (NPG) produced by dealloying possesses a self-organized, self-supporting three-dimensional (3D) nano-architectures, which gains increased attentions as a multifunctional material for a wide range of applications. Similar to small gold nanoparticles, NPG has been demonstrated to be catalytically active for a number of important chemical/electrochemical reactions, but at a much larger characteristic size (>20 nm) for both gold ligaments and nanopores. While many factors have been suggested to explain the nano-size chemical effect of gold nanoparticles, such as quantum size effects, charge transfer between gold nanoparticles and oxide supports, and enhanced concentration of low-coordination atoms, on the other hand the self-supported NPG indicates that the unique morphological characteristics alone is responsible for the catalytic activity of NPG.

We characterized the microstructure of NPG using spherical-aberration-corrected transmission electron microscopy (Cs-corrected TEM). The atomic structure of the internal surfaces of NPG, responsible for the catalytic activity, was imaged by scanning transmission electron microscopy (STEM) using a high-angle annular dark-field (HAADF) detector. The arrangement of near-surface atoms was also measured accurately by Cs-corrected high-resolution TEM (HRTEM), which provides phase-contrast images with high displacement sensitivity. On the basis of extensive HRTEM and STEM characterization, the high catalytic performance of NPG was suggested to originate from surface strains and a high concentration of low-coordination atoms stabilized by the complex geometry of bicontinuous nanoporosity of NPG. In addition to the static observation in inert vacuum environment, we also characterized the surface atomic structure evolution during CO oxidation in a reactive atmosphere using a newly dedicated environmental HRTEM [1].

Our key observation also provided the first direct atomic observations of the coarsening process of the porous catalyst, which shows completely different mechanisms of catalytic degeneration when compared to conventional nanoparticulate catalysts. More importantly, the atomic observation provides compelling evidence that planar defects such as twins can effectively prevent structure coarsening, suggesting a new strategy for developing chemically active and structurally sound catalysts. The effect of planar defects on catalysts has been highlighted recently and our observation offers the first direct experimental evidence of this important phenomenon [2].


Low temperature, hydrogen-fueled, proton exchange membrane fuel cell (PEM-FC) based engines are being developed rapidly for near-term implementation in mass production, personal automobiles. Materials and process research aiming to further optimize these systems is focused on understanding and controlling various degradation processes (carbon corrosion, Pt migration, cold start), and reducing cost by reducing or eliminating Pt in the electro-catalyst, especially for the oxygen reduction reaction (ORR). We are using soft X-ray scanning transmission X-ray microscopy (STXM) at the S 2p, C 1s, O 1s and F 1s edges to study a variety of issues related to optimization of PEM-FC materials for automotive applications. STXM provides spectroscopic identification and quantitative mapping of chemical components within 30 nm spatial resolution in both 2D projection and 3D spectromicroscopy. Themes of our studies include: mapping ionomer in cathodes of beginning-of-life and end-of-life membrane electrode assemblies [1, 2, 3]; investigating Pt-in-membrane [4] and carbon corrosion degradation [3]; studies of alternate electrode technologies (3M nanostructured thin films [5], ink-jet print [6]); and measuring water distributions in situ [7]. The O 1s spectra of the 3 phases of water differ from those of membrane electrode assemblies (MEA) constituents allowing direct in-situ visualization of water uptake and quantitative mapping of gas and liquid/sorbed water. A newly developed environmental cell for in situ studies with controlled humidity and temperature will be described and its current performance will be outlined.

Research funded by AFCC and NSERC. Measurements were made at the Canadian Light Source (supported by NSERC, NRC, CIHR, and the University of Saskatchewan) and at the Advanced Light Source (supported by the Division of Basic Energy Sciences of U.S. DoE).


Over the last several years massive Argon gas cluster ion sources as accessories for sputter depth profiling of organic materials have increased in popularity. These sources utilize Argon cluster ions formed via adiabatic isentropic expansion of Argon gas into a vacuum followed by subsequent electrostatic energy acceleration. In this talk the aforementioned massive cluster ions efficiently sputter the surface of organic materials revealing undamaged subsurface structure for analysis. More recently, developments in the technology have expanded the use of these sources to allow for the sputtering of inorganic materials. Advanced software controlled ion sources and flexible sample handing equipment allow a wide range of experimental conditions to be routinely employed during sputter depth profiling with these massive Ar clusters. In this talk we will demonstrate that, although preferential Oxygen sputtering can be observable for sputtering of inorganic materials where typically high beam energies (typically less than 10keV) are very effective for sputtering of no observable chemical damage. This is in contrast to sputtering of inorganic materials where typically high beam energies (greater than 10keV) and small cluster sizes are required for effective sputtering. The identification of a minimum partition energy for sputtering will be discussed. In addition, it will be demonstrated that, although preferential Oxygen sputtering can be observed on many oxides resulting in the formation of reduced chemical states, this effect is substantially reduced when compared to the use of monoatomic Ar ions.
especially critical when operating electrodes (typically, semiconductors) are exposed to aqueous electrolytes [2]. Therefore, it is desirable to understand the process of water interactions with semiconductors and possible oxidation and reduction mechanisms at the H₂O/semiconductor interface, especially under near realistic conditions.

In the present study, water dissociative adsorption on a GaP (111) surface was investigated using near ambient pressure X-ray photoelectron spectroscopy (NAP XPS) at various pressures and temperatures. The interfacial chemistry was tracked by recording high resolution photoemission spectra of Ga 2p, O 1s and P 2p. In the pressure-dependent study (room temperature, ~300 K), enhanced surface Ga hydroxylation and oxidation were observed with an increase of water vapor pressure, which was also mirrored by the photoemission spectra of O 1s. In the temperature-dependent study, surface Ga hydroxylation and oxidation were further enhanced at temperatures below 673 K. While a large-scale conversion of surface O-Ga-OH species into Ga hydroxide, along with surface P oxidation, was observed at a temperature of 773 K. The formation of Ga and P oxide/hydroxide networks with a schematic formula of GaₐP₇O₇(OH)₃ (ₐ,  b,  c and d represent a ratio of different elements and groups) is suggested. Our results can be compared with recent theoretical findings [3, 4] and lead to a better understanding of water splitting mechanisms and photo-corrosion on semiconductor surfaces.

Reference
Energy Harvesting & Storage Poster Session

EH-WeP1 Lifetime Prediction of Encapsulated Organic Photovoltaic Modules in Accelerated Conditions, SangHwan Kim, N. Kim, Korea Electronics Technology Institute (KETI), Republic of Korea

Organic photovoltaic (OPV) modules consisting of ITO/ZnO/photoactive layer/PEDOT:PSS/Ag inverted structure were fabricated using slot-die coating method and encapsulated by a barrier film deposited on polyethylene terephthalate (PET). Effective water vapor transmission rate was measured in both the transient and steady-state regimes of PET with a barrier film. Acceleration tests were conducted under 65% and 85% relative humidity to investigate the degradation of OPV modules. Total amount of water vapor into OPV module was calculated and correlated with the degradation rate of it. The lifetime of encapsulated OPV module under ambient condition is calculated and will be presented in the conference.

EH-WeP2 Effect of Surface Roughness on the Contact Resistance between the Gas Diffusion Layer and Bipolar Plate in a Polymer Electrolyte Membrane Fuel Cell, Changhee Choe, J.J. Lee, Seoul National University, Korea, Republic of Korea

In a polymer electrolyte membrane fuel cell (PEMFC), one of the most important factors affecting the performance is ohmic loss arising from the contact resistance at the interface of the gas diffusion layer (GDL) and bipolar plate (BP). As a method to reduce the contact resistance between the bipolar plates and gas diffusion layer, the contact area of the bipolar plates were increased by roughening the surface. The environment of the highly porous GDL being pressed by an external compaction pressure was simulated, and the contact area between the GDL and bipolar plates was calculated. The calculated contact resistance using the contact area was compared with the experimental contact resistance results of the bipolar plates polished with various grades of abrasive paper. As the average surface roughness increased, the contact resistance values decreased, which is in good agreement with the results of this study. In a single cell test, the efficiency of the cell increases when the rough bipolar plate is used.

EH-WeP3 Fully flexible and Transparent Piezoelectric Touch Sensor is based on ZnO nanowires with BaTiO3, Moolkyul Kang, J.H. Park, K.I. Lee, Korea Electronics Technology Institute (KETI), Republic of Korea

The ZnO nanowires (NWs) can be grown by chemical approach at low temperature (~100 °C) on any substrate and any shape substrate. A relatively small force is required to induce the mechanical agitation, so that it can be fabricated sensitive devices.[1] But piezoelectric device based on ZnO NWs, which can not improve the piezolectric properties of a single material due to a low piezoelectric d constant of ZnO NWs (d=12pC/N). In this paper, we demonstrated fully flexible and transparent piezoelectric touch sensor based on ZnO NWs, and composed that touch sensor with BaTiO3 of Perovskite structure for improving piezolectric properties. In order to maintain the flexibility of sensing spot, the BaTiO3 (10 wt%) are dispersed in flexibility-improved SiO2 capping solution and coated on ZnO NWs surface as a capping layer by spray coating method. Also, By replacing Indium tin oxide (ITO) electrodes with transparent flexible CNT-Ag nanowires electrode, the flexibility of the entire structure was enhanced. ITO is commonly used as transparent electrodes. However due to its high cost and limited supply of indium, the fragility and lack of flexibility of ITO layer, its alternative are being sought. It is expected that conductive films using carbon nanotubes and Ag NWs could be a prospective replacement of ITOs.

The ZnO NWs based sensor generated the output voltage of ~ 50 mV. The sensor with BaTiO3 generates a higher output voltage (~1.2 V) than a ZnO NWs based sensor. We confirmed that the output voltage of sensor with ZnO NWs and BaTiO3 was dramatically increased. We measured the resistance of capping layer and CNT-Ag NWs electrode during the periodic bending. When bent and flexed over 1,000 cycles, the films did not show significant degradation in sheet resistance compared to Ag thin film and ITO film on the same PET substrate. The bending test results conducted to confirm the mechanical stability of capping layer and CNT-Ag NWs as a electrode. The measurement results suggest that the piezoelectric touch sensors are suitable for flexible device such as flexible touch sensor, wearable and rollable touch panel.


EH-WeP4 Analysis of Steam Reforming Reaction by Vibrationally-Excited Methane Based on First-Principle Molecular Dynamics Simulation, Naoki Tokoyama, Y. Higuchi, N. Ozawa, H. Yagami, M. Kubo, Tohoku University, Japan

For an environmentally-friendly energy system, hydrogen is expected as a resource to replace fossil fuels. Recently, steam methane reforming (SMR) is mainly used for hydrogen production. However, the promotion and the cost reduction of hydrogen production in SMR is strongly desired for stable supply of hydrogen because SMR requires a large amount of heat. To increase hydrogen production, Maegami et al. proposed the vibrationally-excited light, in which infrared light vibrationally excites a CH bond of a CH4 molecule[1]. While hydrogen production is promoted by the vibrational excitation of a CH4 molecule, the detailed analysis at atomic scale is necessary for higher efficient hydrogen production. Thus, by using the first-principles molecular dynamics (FPMD) simulation method, we examined the effect of vibrational excitation of the C-H bond on chemical reaction dynamics for hydrogen generation from CH4 and H2O.

To reveal the chemical reaction dynamics, we simulated collision process of a H2O molecule with a CH4 molecule in the vibrationally-excited state by using our development FPMD code “Violet”[2]. The vibrationally-excited state was reproduced by extending a C-H bond. After the collision, a dissociation of C-H bond was observed. Moreover, the H atom of the dissociated C-H bond reacted with a H atom of the H2O molecule, and H2 and CH3OH were generated. Next, to examine the effect of vibrational excitation, we simulated collision processes with the collision angle from -60° to 60° and collision energy from 9 eV to 20 eV. In the ground state, hydrogen molecules were generated in the range of collision angle from -50° to -10° and collision energy from 17 eV to 20 eV. On the other hand, in the vibrationally-excited state, hydrogen molecules were generated in the range of collision angle from -60° to 0° and collision energy from 14 eV to 20 eV. Therefore, in the vibrationally-excited state, H2 molecules were generated in a wider range of collision angle and lower collision energy than those in the ground state. This simulation result suggests that the H2 generation was promoted by vibrational excitation, which is consistent with the experiment[1]. We also examined the later process after the H2 and CH3OH were generated. Accordingly, CH3OH, CH2O, H2COOH, and CO were observed as intermediate products. Consequently, we indicated the chemical reaction dynamics of H2 generation from H2O and vibrationally-excited CH4 in gas phase.


EH-WeP7 The Integration of XPS and Ar-Gas Cluster Ion Sputtering to Study the Corrosion of Stainless Steel Surfaces, D. Surman, Kratos Analytical Ltd., Helen Brannon, J. Counsell, S. Hutton, Kratos Analytical Ltd., UK, J. Morrison, University of Birmingham, UK, C. Blomfield, Kratos Analytical Ltd., A. Roberts, Kratos Analytical Ltd., UK

Stainless steels are vital construction materials in all areas of industry, combining excellent corrosion resistance with good mechanical properties. For these reasons, stainless steels are used extensively in power stations of all varieties – of particular interest is the use of stainless steel in Pressurised Water Reactor (PWR) type nuclear power plants, such as the Sizewell B power station, Suffolk, UK. The corrosion of steel in contact with hot, pressurised water in a PWR is a common problem. This side reaction is undesirable due to the reduced heat transfer efficiency caused by the deposited oxide layers.

Stainless steel’s corrosion resistance is derived from the formation of a passivation layer at the surface of the material. Under atmospheric conditions this is thought to be a vanishingly thin layer of Chromia (Cr2O3), however, under conditions found in the coolant cycles of a PWR, it is thought that the passivation layer grown forms a double layer – the inner layer consisting of corrosion resistant, non-stoichiometric Chromite (FeCr2O4), while the outer layer consists of non-stoichiometric Nickel Ferrite (NiFe2O4). The thickness of this film is believed to vary with the steel surface finish, and the Environment Degradation Group at the University of Birmingham has recently begun a programme to study the dependence of corrosion rate and passivation layer thickness on surface finish, system chemistry and temperature.

The samples were ground to a 120 and 1200 grit finish using silicon carbide paper to produce samples with significantly different roughness levels.
EH-WeP9  Current Enhancement in Hybrid Solar cells prepared with Quantum Dots and PFN, D. Esperanza, J. Oliva UC, T. Lopez, I. Zarazua, Elder De la Rosa, Centro de Investigaciones en Optica A.C., Mexico

This work presents a hybrid solar cell made with quantum dots and poly [(9,9-bis(3′-(N,N-dimethylamino)propyl)-2,7-fluorene)-alt-2,7-(9,9-diocetylfluorene)] (PFN), which is commonly used as electron transport layer in organic solar cells. Those cells were fabricated by Successive Ionic Layer Adsorption and Reaction (SILAR) method and spin coating. The configuration used in this work was: TiO2/PbS/PFN/CdS/ZnS. The presence of PFN produced an increase of 33% in the short circuit current (JSC) respect to the sample of reference: TiO2/PbS/CdS/ZnS. The presence of PFN produced an increase of 33% in the short circuit current (JSC) respect to the sample of reference: TiO2/PbS/CdS/ZnS. The increase in current caused an increment of the cell efficiency from 2.6% to 3.6%. PTB7 was also used has donor in our hybrid solar cells instead of quantum dots, when the PFN is added in this system, the current increased 60% respect to the cell of reference and the efficiency increased from 1.1% to 3.0%.

EH-WeP11  On the Role of Plasma System for CO2 Dissociation, H.Y. Chang, Korea Advanced Institute of Science and Technology (KAIST), South Korea

The CO2 capture and storage technology (CCS technology) needs immediate action, but does not have complete solutions yet due to the governing fundamental quantities will be identified to obtain the maximum energy efficiency and capacity for CO2 dissociation. Several CO2 conversion ideas will be introduced, describing the advantages and disadvantages of each conversion techniques. The plasma reactor has been known as one of the most promising candidate for CO2 dissociation. The plasma reactor and chemical discharge at atmospheric pressure, and reliability at high power density should be solved. The ICP (Inductively coupled plasma) source will be introduced along with other sources such as microwave, DBD (Dielectric barrier discharge), and DC for the efficient CO2 dissociation. In this presentation, the technical issues for the mass production of CO2 conversion will also be discussed.

EH-WeP15  Positive Temperature Coefficient of CdS/Cu(In,Ga)(S,Se)2 Solar Cell, Sangmom Kim, C.-W. Jeon, Yeungnam University, Republic of Korea

In the recent years, Cu(In, Ga)Se2 (CIGS)-based thin-film solar cells with efficiency of readily over 20% have been reported by several groups, therefore, it is strongly expected to replace the crystalline silicon solar cell rapidly. Unlike crystalline silicon cell of a homo-junction, CIGS thin-film solar cell consists of hetero-junction between absorbing layer and CdS buffer layer. In CBD (Chemical Bath Deposition)-CdS, which is commonly used for high efficiency CIGS solar cell, the kind and concentration of source materials and bath temperature is known to affect the characteristics of the CIGS/solar cell as well as CdS film properties. In general, the efficiency of solar cell decreases with increasing ambient temperature due to the reduction of band gap energy of absorber layer and higher reverse saturation current at an elevated temperature. In other words, temperature coefficient (TC) of a solar cell is normally negative. While this tendency is observed in the CIGS/CdS solar cells, according to this study, it was confirmed that the behavior of TC depends on the synthesis conditions of the CdS. In this study, we prepared several solar cells of ZnO/CdS/CIGS/Mo/glass with different CdS deposition conditions by changing [Cd] and [S] in the solution over the range of [Cd]=15–135 mM, [S]=12.5–540 mM. And the variation of TC’S were monitored by measuring IVT (Current-Voltage-Temperature) at temperature range of 10–50°C. Some of solar cells with high [Cd] of low [S] were found to have positive TC’S. In these devices, while Voc decreased as expected with increasing temperature, fill factor increased on the contrary. The enhancement of fill factor stemmed from the lower series resistance at higher operating temperature.
On this work we study the formation of gold NPs by thermal and laser annealing, without studying the evolution of the process in time; notwithstanding the annealing time. For the case of thermal annealing, the NPs size strongly depends on the interval of time in which the sample is inside the oven. In studies mainly focuses on the resulting final crystallography was analyzed by X-ray diffraction (XRD). Hydrogen permeation test of samples, 35 mm diameter and 0.1 mm thick, was conducted at 773K. The fine-grained and (111) oriented TiN film whose grain size was under 100 nm reduced hydrogen permeation by three orders of magnitude compared to untreated stainless steel. Grain interface was thought to be effective hydrogen trap sites.

The hydrogen permeation behavior of thin films coated Type 316L stainless steel was investigated. Thin films of TiN, TiC, Al2O3 were deposited by ion plating. Coated samples were examined using optical microscopy and scanning electron microscopy (SEM). The coating chemistry was determined using Energy Electron Probe Micro Analysis (EPMA) and the crystallography was analyzed by X-ray diffraction (XRD). Hydrogen permeation test of samples, 35 mm diameter and 0.1 mm thick, was conducted at 773K. The fine-grained and (111) oriented TiN film whose grain size was under 100 nm reduced hydrogen permeation by three orders of magnitude compared to untreated stainless steel. Grain interface was thought to be effective hydrogen trap sites.

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mobility of exciton mobility and device performance. In addition, we have found that the charge transfer region where carriers efficiently pass from donor to acceptor is approximately one monolayer wide, significantly narrower than was previously believed. This understanding is possible through the examination of electron density and chemical modifications in the molecular species which we observe using the FSRS technique in thin film samples for the first time.


We demonstrate an in-depth characterization of local opto-electronic properties in hybrid organic-inorganic perovskite materials for solar cells using complementary scanning probe techniques.

Perovskite solar cells have the potential to combine high efficiency and low-cost fabrication compared to other third-generation solar technologies; Since 2009, power conversion efficiency of perovskite solar cells has rapidly increased from 3.8% to almost 20%. However, one of the main challenges to systematically increase power conversion efficiency and to develop cost efficient fabrication techniques is the lack of understanding of the exact operating mechanism in perovskite solar cells. In particular, the relationship between morphology, chemical composition, and optoelectronic processes and their impact on overall performance in these materials is hardly understood.

We have studied two promising solution processed hybrid organic-inorganic perovskite materials, CH₃NH₃PbI₃ and CH₃NH₃PbI₃-xClₓ, using scanning probe techniques to determine local photocurrent generation, topography, and the local electronic structure. Depending on composition and fabrication approach, we observed substantial differences in local morphology, crystallinity, photocurrent generation, and photoluminescence. Specifically, we have measured a significant heterogeneity in the local photocurrent generation that does not correlate with topography but rather with the local electronic structure.

8:40pm EH-WeE10 Oxide Heterojunction Electrodes for Sunlight Conversion and Storage, S. Kim, Hyunwoong Park, Kyungpook National University, Korea

TiO₂ and WO₃ heterojunction electrodes are studied for their bi-functionality on harvesting light and storing energy. Both semiconductors are fabricated either ‘single’ (mixed) electrodes or two different electrodes galvanically coupled in a mixed electrolyte of 0.1 M sodium formate and 0.1 M sodium chloride. Irradiation of AM 1.5-light shifts the open circuit potentials (OCPs) of the mixed and coupled electrodes from around – 0.1VSCE (dark OCPs) to a potential range between – 0.8 and – 0.5VSCE, which slowly return to their respective dark OCPs over a period of around 14 hours. Such discharging periods are significantly influenced by the irradiation (photocharging) time and weight or area ratios of TiO₂ and WO₃. When the TiO₂ and WO₃ mixed electrodes are galvanically coupled to stainless steel electrodes for application to anticorrosion, the mixed potentials of the couple are maintained at ca. – 0.4 VSCE over 10 hours even after light off. The measured galvanic currents verify that the photogenerated electrons of TiO₂ flow to WO₃ (charging) and even overflow to the steel (cathodic protection) during the irradiation, while the stored electrons at WO₃ flow to the galvanically coupled steel electrodes directly or through the TiO₂ upon light off. This research was financially supported by the Basic Science Research Program (NRF-2012R1A2A2A01004517) and Frame-work of International Cooperation Program (NRF-2013K2A1A2052901).
8:00am EH-ThM1 Improving the Photoconversion Efficiency of Quantum Dots Sensitized TiO2 Solar Cells Prepared by SILAR and Electrophoresis Method, I. Zarazua, Centro de Investigaciones en Optica, León, D. Esparza, A. Sanchez, A. Cerda, T. Lopez-Luke, Elder De la Rosa, Centro de Investigaciones en Optica A.C., Mexico INVITED
One of the most studied hybrid-type nanostructured solar cells is the Gratzel or dye sensitized solar cell (DSSC). DSSCs typically consist of TiO2 NCs acting as a highly porous, wide bandgap semiconductor for electron collection, and dye molecules adsorbed onto the TiO2 NCS surface acting as sensitizers to harvest solar light. An alternative to DSSC is the utilization of quantum dots (QDs), e.g., CdSe, CuTe, CsS, PbS, PbSe, Bi2S3, and InP, as sensitizers to replace the expensive ruthenium dyes. QDs have large extinction coefficients in the visible region and, after bandgap excitation, undergo charge separation, injecting electrons to the conduction band of the metal oxide
The quantum dots (QD) has been recently drawing great attention as a material for solar energy conversion. The quantum dots sensitized titanium dioxide (TiO2) was synthesized by different chemical methods such as successive ion layer formation and electrodeposition and their performance in electrochemical and photoelectrochemical (EP) studies. Today, the use of QDs sensitized solar cells is becoming a research focus for harvesting solar energy due to their large surface area and good charge transfer properties. In this paper, we present a detailed analysis of charge transport on both configurations presented treating vacuum as an impendence spectroscopy (IES) a detailed analysis of each interface is also presented.

We acknowledge financial support from CONACYT through grant 134111, UC-MEXUS program, CEMIE-Sol (P28), and European Community Seven Framework Programme (FP7-NMP-2010-EU-MEXICO) and CONACYT under grant agreements 263878 and 125141, respectively. D. Esparza, Andrea Sanchez and Andrea Cerda acknowledge scholarship from CONACYT.

8:40am EH-ThM3 Applications of pure ZnO and the Mn-doped ZnO on Dye Sensitized Solar Cells, P.X. Feng, Xiaoyan Peng, Y.M. Li, UPR, Puerto Rico
Mn-doped ZnO nanopowders have been prepared by the sol–gel technique using zinc and manganese (II) acetates as precursors. The crystalline structure investigations reveal that as prepared nanocrystals with low Mn doping concentration have single hexagonal phase and are grown along the structural investigations reveal that as prepared nanostructures with low Mn using zinc and manganese (II) acetates as precursors. The crystalline Mn-doped ZnO nanopowders have been prepared by the sol–gel technique. The sol–gel process involves a liquid phase transformation of a sol to a gel through condensation and polymerization reactions.

Aloi

Electrophoresis Method
Quantum Dots Sensitized TiO2 Solar Cells Prepared by SILAR and Electrophoresis Method
8:00am EH-ThM1 Improving the Photoconversion Efficiency of Quantum Dots Sensitized TiO2 Solar Cells Prepared by SILAR and Electrophoresis Method, I. Zarazua, Centro de Investigaciones en Optica, León, D. Esparza, A. Sanchez, A. Cerda, T. Lopez-Luke, Elder De la Rosa, Centro de Investigaciones en Optica A.C., Mexico INVITED
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References:


Results will be reported for the thermodynamic and kinetic constraints on such processes, together with the effects of experimental variables on H₂ production rates.

11:00am EH-ThM10 Gate-Modulated Thermoelectric Characteristics of Silicon Nanowires on Plastic Substrates, Youngin Jeon, Korea University, Republic of Korea, J. Choi, K. Cho, Korea University, S. Kim, Korea University, Republic of Korea

Recently, several novel concepts of thermoelectric technologies have been reported as a promising source of next-generation regenerative energy. Moreover, silicon nanowire (Si NW) based thermoelectric devices are an attractive research area due to their advantages such as non-toxicity, abundance, and low-cost manufacturing, which can lead to new opportunities in broad areas of commercial electronics. The efficiency of energy conversion has been intensively studied by modulating the dimensionless thermoelectric figure of merit, ZT = σS²T/κ, where σ is the electrical conductivity, S is the Seebeck coefficient, κ is the thermal conductivity, and T is the absolute temperature. Numerous studies indicate that the use of Si NW enables the improvement of ZT due to their low-dimensional properties. Nevertheless, it is still difficult to achieve high ZT value because σ, S and κ are interdependent. Therefore, the modification of these parameters in Si NW can enhance the thermoelectric properties. Among various fields of research, applying electric fields on thermoelectric materials, may be one of the prominent ways to modulate the thermoelectric parameters. In this study, we fabricate a gated Si NW thermoelectric device constructed on a thermal-insulating plastic substrate, and examine the field-effect modulation of thermoelectric characteristics.

Figure 1 shows the optical image of our gated thermoelectric device on a plastic substrate. The structure of the device with a NW channel length of 50 μm is similar to a NW field-effect transistor. N-type Si NWs with a doped concentration of 10^{12} cm⁻³ are present between the electrodes and a gate electrode is located at the middle of the Si NWs. And a heater electrode is used as a heating source. We investigate the seebeck voltage variation of the gated thermoelectric device with the gate bias is applied. Figure 2(a) exhibits the seebeck voltage versus temperature variation characteristics of the device with V₉₀₋₀ from 0 to 5 V. Our device shows the good gate controllability of the channel voltage potential, which implies the capability of the electrical conductivity modulation for the Si NWs. Thus, as V₉₀ decreases, the conductivity of the Si NWs also decreases accordingly, leading to the increase of the seebeck voltage with the same temperature variation. Therefore, as shown in Figure 2(b), the seebeck coefficient, defined as −ΔV/ΔT, is able to modulate with the gate voltage variation. Our study suggests that the gated thermoelectric device with n-type Si NWs on a plastic substrate reveals a potential use as a next-generation energy harvesting device.

11:20am EH-ThM11 Transition Metals Ion Implantation into AlN/GaN Thin Films, Abdul Majid, University of Gujarat, Pakistan, Zhu, Chinese Academy of Sciences, Beijing

A lot of work has been done on Mn doping in III-V [1] but work on Mn and other TM ions doping in AlN is still lacking. Out of III-Nitrides, AlN is the only ternary alloy with a capability of lattice matching with GaN and is potential candidate for use as distributed Bragg reflectors, cladding layers and several other electronic /optoelectronic devices[2]. Like several other materials, the doping of AlN with TM elements is expected to produce diluted magnetic semiconductors (DMS) based on it. Realization of AlN based DMS will be exciting due to wide direct band gap and lattice mismatch capability at 17% indium content with GaN. This work is one of the initial detailed reports on TM doping into AlN. Transition metals ions of Cr, Mn, Co and V were implanted MOCVD grown wurtzite AlN/GaN thin films at doses 5x10¹⁴ to 5x10¹⁵ and 5x10¹⁶ ions/cm². The structural properties of the materials were studied by X-ray diffraction and Rutherford backscattering spectroscopy (RBS) techniques. XRD analysis revealed that GaN related peak for all samples remains at its usual Bragg position of 2θ=34.56° whereas a shift in AlN peak taken place from its position of 2θ=35.51° for as-grown sample. RBS analysis provided interesting results with clear shift in position of indium related peak pointing to migration of indium atoms towards interface of heterostructures. Moreover this peak has observed to be splitted into two peaks which is indication of depth wise redistribution of indium atoms within the material. The measurements of magnetic amplitudes versus temperature as well as applied magnetic field measured using SQUID magnetometer indicated room temperature ferromagnetism in the films. The density Functional Theory based calculations of Transition metals doped AlN predicted that TM ions will preferably substitute In sites in the alloy. In order to model the experimental results and explore the mechanism of ferromagnetic exchange interactions in the materials, detailed density functional theory (DFT) based calculations
were performed. The electronic and structural properties of pure and TM doped AlInN were computationally investigated using ADF-BAND program which performs calculations using Kohn-Sham under Local Density Approximation. We modeled 64 atoms supercell with 3x3x3 mesh in the form Al27In5N32 for pure AlInN and Al27In3Mn2N32 (2 Mn atoms substitutes 2 In atoms), Al26In5Mn1N32 (Mn substitutes Al) and Al26In5Mn1N32 (Mn substitutes Al) supercells for Mn doped AlInN. The literature suggests that Fermi level should lie within spin up Mn band predicting Mn:AlInN to be in half metallic state like other Mn doped III-Nitrides [3]. The calculated results indicate that Mn d band is partially filled for Al27In4Mn1N32 and Al27In3Mn2N32 whereas completely empty for Al26In5Mn1N32. It can be said that, either one or two Mn atoms substituting In sites produces expected half metallic AlInN whereas Mn substituting Al sites turns out to be unacceptable option. It is therefore concluded that Mn will preferably substitute indium in AlInN.


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