

Tuesday Afternoon Poster Sessions, July 23, 2019

ALD Applications

Room Evergreen Ballroom & Foyer - Session AA1-TuP

Energy Harvesting and Storage Poster Session

AA1-TuP-1 Study on Atomic Layer Deposited Al₂O₃, TiO₂ and ZnO for the Application in Silicon Photovoltaics, *Arun Haridas, M Sreenivasan*, Hind High Vacuum Company Pvt. Ltd., India; *A Antony*, Indian Institute of Technology Bombay, India

We have fabricated a thermal atomic layer deposition (ALD) system with a substrate size of 150 mm diameter. Non-uniformity of 95 nm Al₂O₃ films deposited over polished (100) Si substrate at a temperature of 200°C is ± 0.41 % over 150 mm diameter as measured using ellipsometry. The optical properties, i.e. n & k values were found to be very uniform indicating the uniformity of the growth and the quality of the layer over large area. Passivation quality of the Al₂O₃ films over the Silicon substrate is studied by measuring the minority carrier life-time and photoluminescence. Application possibility of ALD grown TiO₂ and ZnO films have been examined as carrier selective layer for Silicon.

Highly uniform Atomic layer deposition of Al₂O₃ thin film using trimethyl Aluminium and H₂O as counter reactant has been achieved. Surface recombination is a major loss factor in the Si solar cells. These losses can be reduced with good quality chemical passivation or field effect passivation. Al₂O₃ is a promising high quality passivation material for p-type Si, because of its ability to act as a field effect passivator for the charge carriers. Crucial parameter of this layer is thickness and uniformity that can be precisely controlled using ALD.

The material quality and doping level by the oxygen vacancies of the metal oxide layer plays a crucial role in the performance of the carrier-selective silicon solar cells. High quality films of TiO₂ using Titanium isopropoxide and H₂O, as well as ZnO using diethyl Zinc and H₂O are investigated for carrier selectivity. ALD has very good potential as effective tool for depositing ultra thin carrier-selective layers for solar cells.

In this work we are exploring the advantages of the ALD technique to grow pinhole free, conformal and extremely uniform films for improving the performance of Silicon solar cells.

AA1-TuP-2 Nitrogen-Doped TiO₂ Film Deposited using Plasma-Enhanced Atomic Layer Deposition to Improve the Electrical Conductivity for Surface Passivation of Crystalline Silicon, *E Song*, Korea Institute of Materials Science, Republic of Korea; *J Ahn*, Korea Maritime and Ocean University, Republic of Korea; *Jung-Dae Kwon*, Korea Institute of Materials Science, Republic of Korea

For surface passivation with improved electrical conductivity, we investigate nitrogen doped TiO₂ film by combining the TiO₂, TiN sub-cycles using plasma-enhanced atomic layer deposition. For composition control of the TiON films, a super-cycle was adopted which was composed of one cycle of TiO₂ and x-cycles of TiN. The thickness of the TiON films as the nitrogen doping concentration linearly increases with the number of super-cycles. We confirm the chemical states, crystalline phase and interface characteristics of these TiON films through the XPS, XRD and C-V analysis. When the nitrogen was doped in the TiO₂ thin film, the carrier lifetime was increased from 30 to 243 μs and the resistivity decreased from 3.1E+08 to 7.1E-01 Ω·cm for the TiO₂:TiN=1:20 film.

AA1-TuP-3 Multilayer Encapsulation for Highly Stable Perovskite Solar Cells with Atomic Layer Deposited Al₂O₃ and Chemical Vapor Deposited Flowable Oxide, *Jungwoo Kim, H Hwangbo, S Kim, J Jang, H Tran Vo, H Chae*, Sungkyunkwan University (SKKU), Republic of Korea

Perovskite solar cells (PVSCs) are known to be easily deteriorated in atmospheric environment. Many researchers have studied encapsulation technique to protect PVSCs. However, few researchers reported long term stability under severe conditions such as 85 °C with 85% relative humidity (RH). Atomic layer deposited metal oxides are considered to be effective to thin film encapsulation. However, PVSCs can be easily damaged by oxygen radicals during the metal oxide deposition process. In this work, we introduced flowable oxide inter layer for the cell protection before spatially-resolved plasma atomic layer deposition (ALD) process. The flowable oxide layer prevent oxygen radicals generated in N₂O plasma during Al₂O₃ process and the power conversion efficiencies (PCEs) of PVSCs were almost preserved. With flowable oxide and Al₂O₃ double layer, 45% in efficiency drop was observed after 1000 hours in 85 °C/35% RH condition. The PVSCs with multiple stacked flowable oxide/Al₂O₃ layer with glass encapsulation showed less than 10% of efficiency degradation after 1000 hours in 85 °C/85% RH. The multilayer with flowable oxide protection layer

and Al₂O₃ moisture barrier layer structure is expected to provide long term stability in ambient condition.

AA1-TuP-5 Oxide Buffer Layers for Perovskite Solar Cells Grown with a 200 mm Commercial ALD System Using Low-Temperature Process, *P Rajbhandari, Tara Dhakal*, Binghamton University

Organic materials provide a very small thermal budget for any post-fabrication treatment or for a subsequent layer in device fabrication. The demand for the low-temperature process has driven the focus of our study to obtain atomic layer deposited oxide buffer layer at temperatures suitable for a perovskite solar cell. The buffer layer will assist in blocking holes, effectively extract electrons, provide better shunt protection and act as a sputter protection layer covering the organic perovskite films from sputter damage from a subsequent layer, such as a transparent conductor. Three different oxide layers, Al₂O₃, ZnO, and TiO₂ are grown at 100°C and studied for this purpose using **Synchronous Modulated Flow Draw ALD (SMFD-ALD)** technology optimized in commercial 200 mm ALD reactor from Sundew Technologies. It allows greater precursor utilization and shorter deposition cycle times that in turn reduces thermal processing time compared to traditional ALD processes. These thin films have shown to enhance the fill factor (FF) and high charge extraction from the solar cell. Three oxides are compared on all aspect, among which ZnO (4 nm) along with Al₂O₃ (1 nm) as a buffer layer has shown excellent performance improvement in the device up to 20% power conversion efficiency. In this presentation, ALD growth details of the oxide layers and the resulting perovskite solar cell results will be discussed.

AA1-TuP-6 Ultra-thin Nickel Films for Energy Harvesting Applications, *Ken Bosnick, P Motamedi*, National Research Council Canada, Canada; *K Cadien*, University of Alberta, Canada; *K Harris, J Cho*, National Research Council Canada, Canada

The harvesting of ambient heat and light could potentially lead to useful power for driving off-grid, internet-of-things sensors. Recent theoretical predictions suggest that ultra-thin Ni films can show thickness dependent optical properties that can lead to enhanced solar absorptance. The maximum solar absorptance is predicted to occur at a very thin layer thickness of ~12 nm and is attributed to an impedance matching effect [N. Ahmad, *et. al, Nano Energy* **1**, 777 (2012)]. Light absorptance in ultra-thin Ni films can be further enhanced by patterning the Ni films and depositing multi-layer structures. Atomic layer deposition (ALD) produces conformal films with a high level of control and uniformity with respect to the film thickness. While ALD is most widely known for depositing ultra-thin dielectric materials for advanced electronics applications, we have successfully used the technique to deposit ultra-thin Ni films [P. Motamedi, *et al., ACS Appl. Mater. Interfaces* **9**(29), 24722 (2017); P. Motamedi, *et al., Adv. Mater. Interfaces* **5**(24), 1800957 (2018)].

In this study, ALD Ni films are deposited with varying thicknesses onto fused silica and sapphire substrates. Structural characterization indicates that the films are continuous, polycrystalline Ni films with a relatively low degree of roughness and are suitable for comparison with the theoretical predictions. Optical absorptance is measured using an integrating sphere as a function of film thickness and compared with theory. An optimum thickness is found but the experimentally determined absorptance maximum is less significant than theoretically predicted. Possible explanations include surface roughness or deviations from the refractive index of bulk Ni. Nevertheless, the thickness for optimum absorptance is found to be around 10 nm for planar ALD Ni films.

Glancing angle deposition (GLAD) is used to produce quasi-periodic silica pillars on fused silica wafers and ALD Ni films are deposited conformally onto the GLAD pillars. It is hypothesized that the GLAD films with ultra-thin ALD Ni coatings will act similarly to lithographically patterned gratings and lead to enhanced optical absorptance. Optical absorptance measurements reveal a low reflectance at all wavelengths, but an extremely high absorptance in the UV / visible range that decreases to very low values in the NIR. The spectra are seen to have a strong dependence on the ALD Ni thickness but to be less sensitive to changes in the GLAD deposition parameters. Structural characterization, further control experiments, and theoretical modeling are planned to understand these optical results.

AA1-TuP-7 MoNx-Deposited on High-surface N-doped Carbon Coated-Carbon Cloth Substrates: The Best Possible Option for ALD in View of Energy Storage Application, *S Sawant, D Nandi, R Rahul, S Kim, Moo Hwan Cho*, Yeungnam University, Republic of Korea

Molybdenum [https://www.sciencedirect.com/topics/chemistry/nitride] (MoN_x) was directly grown on 3-dimensional nitrogen doped-carbon coated

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carbon cloth (NC-CC) at a relatively low temperature of 250 °C by atomic layer deposition (ALD) and then tested as an electrode for supercapacitive charge storage. The charge storage performance of NC-CC and MoN_x deposited CC have also been evaluated for the comparative studies. The successful formation of MoN_x@NC-CC and MoN_x@CC composite was confirmed by several characterization techniques. The scanning and [https://www.sciencedirect.com/topics/chemistry/transmission-electron-microscopy] analyses showed the extremely uniform and conformal coating of the MoN_x on NC-CC. The 3D and porous texture of NC provided the excessive surface area for MoN_x coating and also granted easy access for the electrolyte penetration. The high areal capacitance of 911 mF/cm² was achieved at a current density of 4 mA/cm² which is 1.3 times higher than that of NC-CC. The negligible charge storage capacity of 7 mA/cm² obtained for MoN_x@CC highlighted the significance of NC deposition on CC prior to the loading of MoN_x. The ultra -high stability of MoN_x@NC-CC (108% capacity retention after 50,000 cycles) further confirmed its exceptional supercapacitive charge storage performance.

AA1-TuP-8 ALD Coatings for Nano Imprint Masks, Thomas Seidel, Seitek50
Nano Imprint Lithography (NIL) usage has been limited by mask defects during fill and release process steps. Additionally, as for any process step, it is desirable to improve throughput. The optical intensity in the features of quartz imprint masks with high index conformal coatings was simulated using Maxwell solver software.¹ The index of refraction of the coatings, exposure wavelength, aspect ratio, film thickness and feature size were varied parameters. The simulations indicate the optical intensity may be increased within the mask features using coatings of higher index films relative to the uncoated reference quartz mask for physical feature sizes below 7nm, indicating the possibility of improved productivity.² Defectivity is proposed to be addressed by the application of *fractional* fluorine terminated monolayers of a fluoro-hydrocarbon (FHC) film at the mask feature surface. This approach is intended to address the dichotomy of fill and release type defects in the imprint feature.^{1,2} In addition, ALD conformal films may be used to reduce the critical feature size below that achievable with the state-of-the-art electron beam processes. A matrix of candidate ALD precursors and processes for higher index coating films (Al₂O₃, TiO₂ and Si) relative to quartz, as well as monolayer FHC precursors are reviewed with considerations of quality and throughput. Various ALD wafer systems are considered for process deposition for square mask quartz plates of 6in. x 6in. x 0.25in. geometry.

The support of Nayoa Hayashi and Nobuhito Toyama of Dia Nippon Printing is acknowledged for the simulations.

1. T. E. Seidel, A. Goldberg and M. D. Hall; "Optical Simulations for Fractional Fluorine Terminated Coatings on Nanoimprint Lithography Masks," *Proc. SPIE* 9635, Photomask Technology 2015, paper 963505 (October 23, 2015)

2. Thomas E. Seidel US 10,156,786B "Method and Structure for Nanoimprint Lithography Masks using Optical Film Coatings," Dec 18, 2018

AA1-TuP-9 The Investigation of Al₂O₃ Passivation Characteristics in the Condition of Growth Temperature and Ozone Concentration, Young Joon Cho, H Chang, Chungnam National University, Republic of Korea

The surface passivation for high efficiency c-Si solar cell is a prerequisite for the achievement of high efficiency solar cell. The capability of Al₂O₃ passivation using trimethylaluminum(TMA, Al(CH₃)₃) precursor and H₂O oxidant was presented. Aluminum oxide (Al₂O₃) grown by atomic layer deposition (ALD) was showed excellent passivation performance as good as obtained by thermally grown SiO₂. A superior property of the ALD- Al₂O₃ film appeared to be the field-effect passivation induced by negative fixed charges and the high level of chemical passivation resulting from a low interfacial defect density. ALD- Al₂O₃ film using ozone oxidant showed better thermal stability and no-blistering because of excluding hydroxyl group in ozone oxidant. Therefore, more detail study is required about the effect of growth temperature and ozone concentration on ALD- Al₂O₃ passivation.

Al₂O₃ were deposited on 8 inch p-type crystalline semiconductor Si(100) wafers of 10 Ω-cm resistivity and 710 ~ 740 μm wafer thickness. Al₂O₃ films of about 20 nm thickness were deposited in the range of 150°C and 300°C with trimethylaluminum (Al(CH₃)₃) (TMA) precursor and ozone oxidant at the concentration of 200g/Nm³ and 330g/Nm³ after RCA cleaning. Comparing H₂O oxidant, ozone oxidant has several advantages, such as its higher activity for ligand elimination relative to H₂O, significantly less amount of defect states like Al-Al and OH bonds compared with those prepared with H₂O. Ozone concentration was controlled by MKS ozone generator at 150g/Nm³ (~10wt%) and 330g/Nm³(~20wt%).

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As a result, the lifetime and implied Voc for the as-deposited Al₂O₃ shows the maximum at growth temperature 250°C and for both of ozone concentration 200g/Nm³ and 330g/Nm³. After annealing, the lifetime and implied Voc has a similar tendency with the as-deposited Al₂O₃. We investigated the reason that the lifetime and implied Voc have a maximum at 250°C before and after annealing through SIMS(secondary ion mass spectroscopy), XPS(X-ray photoelectron spectroscopy), TEM(tunneling electron microscopy), etc.

AA1-TuP-10 Effect of Al₂O₃ Passivation on n-type Si Solar Cell with Passivated Emitter and Rear Cell (PERC), Kiryun Kim, H Chang, Chungnam National University, Republic of Korea

N-type solar cells are immune to LID (Light Induced Degradation) effect, because of the absence of the boron-oxygen defect. However, The fabrication process of n-type PERC includes more steps and makes a solar cell more expensive. Therefore, newer technologies will be needed efficient process steps and structures.

In this study, we investigated n type-PERC cell formed by double-sided Al₂O₃ deposition using ALD. Al₂O₃ films as a passivation layer were grown by ALD at 300°C. After double-sided Al₂O₃ deposition, UV laser ablation with ns pulse performed to make a electrode contact-patterning. Finally, we evaluated passivation performance as a function of emitter sheet resistance and electrode open ratio. In addition, we have evaluated the passivation characteristics affected by electrode materials such as Cu and Al.

The passivation performance of the Al₂O₃ layer was compared with the emitter saturation current (J₀) and the implied Voc through Quasi-Steady-State Photoconductance (QSSPC). As a result, We have achieved iVoc of 680 mV through the optimization process.

AA1-TuP-11 High Quality CaF₂ from a New ALD Process: Enabling New Approaches in Battery Technology and Optical Applications, Max Gebhard, A Mane, J Elam, Argonne National Laboratory

Calcium fluoride (CaF₂) is highly transparent over a broad range of the electromagnetic spectrum, covering ultra-violet (UV), visible, and infrared (IR) wavelengths. Its high transparency between 150 nm – 12,000 nm and its extremely low refractive index *n* (~1.43 at λ = 500 nm - 600 nm) makes it a well-known candidate for optical applications. In combination with materials exhibiting a higher refractive index, CaF₂ coatings find application in anti-reflective coatings and band pass filters. Like other fluorides, such as MgF₂ and LaF₃, the ionic bonding situation in CaF₂ enables applications even below 200 nm (*e.g.* photolithography). Recently, metal fluoride materials were also suggested to be incorporated in Lithium-Ion-Batteries, acting either as the solid electrolyte or electrode material.^[1]

In both cases, *i.e.* optical applications (such as lenses and three-dimensional structures for optical filters) and coatings in Li-ion batteries, the respective thin film must be of high purity and thickness control is of utmost importance. In consequence, the fabrication of CaF₂ via ALD is the method of choice. Different ALD processes for CaF₂ have been reported in the past, using Ca(thd)₂^[2,3] and Ca(hfac)₂^[4] as metal source and NH₄F,^[2] TiF₂,^[3] and Hhfac^[4] as fluorine precursor.^[2] These processes showed best results at temperatures around 300 °C.

Herein, we present a new and straight-forward ALD process for CaF₂ thin films using the [Ca(amd)₂]₂-dimer and HF-pyridine as precursor, working at temperatures as low as 175 °C. The process was monitored and optimized employing *in-situ* diagnostics such as FTIR and QCM, and thin films were characterized in terms of their composition (XPS), structure (TEM, XRD, PDF) and optical properties (UVVis, ellipsometry). The process was applied to cathode powers used in Li-ion-batteries and the performance of the respective materials was investigated.

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AA1-TuP-12 Properties of Molybdenum Oxide Deposited by Plasma Enhanced Atomic Layer Deposition for High Efficiency Solar Cells, Taewan Lim, H Chang, Chungnam National University, Republic of Korea

Transition Metal Oxides (TMO) are applied as a carrier selective contact layer in silicon hetero junction (SHJ) solar cells. MoO_x has high work function (> 6 eV) and wide band gap (~ 3 eV). It is well known that molybdenum oxide exhibits good optical and electrical properties when deposited on Crystalline Silicon (c-Si). But, MoO_x is sensitive to

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temperature, plasma, and air exposure, and for this reason the work function of MoO_x is degraded and its properties are reduced.

In this study, MoO_x is deposited by plasma-enhanced atomic layer deposition (PE-ALD) using Molybdenum hexacarbonyl (Mo(CO)₆) is selected as precursor for Mo and O₂ is adopted as precursor for plasma. Argon was used as a carrier gas of Mo(CO)₆ and the gas line and canister temperature was maintained to 40°C and 45°, respectively. To obtain the best passivation performance, the plasma power was varied between 10W and 500W at PE-ALD process. To investigate the effect of temperature, the sample was annealed at temperature range from 250 °C to 500 °C.

X-ray photoelectron spectroscopy (XPS) analysis confirmed the chemical state of the MoO_x film. The growth per cycle (GPC) of MoO_x film and MoO_x/c-Si interface was investigated by transmission electron microscopy (TEM). The GPC of MoO_x film deposited by PE-ALD was found to be 0.25 Å. The life time and V_{oc} were measured by quasi steady state photoconductivity (QSSPC).

AA1-TuP-13 Understanding and Mitigating F Migration in ALD Nanocomposite Coatings, Anil Mane, M Gebhard, J Elam, Argonne National Laboratory; M Popecki, T Cremer, Incom Inc.; M Minot, incom

We have developed atomic layer deposition (ALD) processes to synthesize metal-dielectric oxide nanocomposite coatings comprised of conducting, metallic nanoparticles (M) embedded in an amorphous dielectric matrix, nominally Alumina (Al₂O₃), and where the metallic component is selected from either tungsten (W) or molybdenum (Mo). The nanocomposite layers are prepared using alternating exposures to trimethyl aluminum (TMA) and H₂O for the Al₂O₃ ALD and alternating metal hexafluoride / disilane (MF₆/Si₂H₆) or metal hexafluoride TMA (MF₆/TMA) exposures for the metal ALD component. By varying the ratio of M:Al₂O₃ ALD cycles and the order of precursor dosing for the two components, we can tune the composition enabling a wide range of mechanical, electrical, and optical properties of these nanocomposites. We have applied these nanocomposites to a variety of applications, but I will focus this presentation on their use as resistive layers for glass capillary array microchannel plates (GCA-MCPs). These ALD nanocomposite coatings contain residual fluorine (F) from the metal hexafluoride precursor in the form of AlF₃. Although we can modulate the F content by adjusting the W nucleation conditions, it is not possible to eliminate the F and this can introduce challenges for device fabrication and integration. For instance, we often deposit ALD magnesium oxide (MgO) following the ALD resistive coating to improve the secondary electron emission (SEE) of the surface. In these cases, we find that residual F can diffuse from the resistive layer into the MgO forming MgF₂ and affecting MCP performance. In this presentation, I will describe several strategies we have developed to minimize F migration. I will conclude by showing the enhanced performance and stability of ALD-GCA-MCPs achieved with this technology.

AA1-TuP-14 Ultrathin Metal Oxide Passivation by Atomic Layer Deposition Enhances Stability and Performance of Visible Solar Water Splitting on Solution-Processed Organic Semiconductor Thin Films, L Wang, D Yan, Stony Brook University; D Shaffer, Brookhaven National Laboratory; X Ye, Stony Brook University; B Layne, J Concepcion, M Liu, Chang-Yong Nam, Brookhaven National Laboratory

Solution-processable organic semiconductors have potentials for visible photoelectrochemical (PEC) solar water splitting because of their tunable small band gaps and electronic energy levels. However, the poor stability and photocatalytic activity of organic semiconductors have been posing persistent challenges. Here, we demonstrate that the application of ultrathin metal oxide passivation by low-temperature atomic layer deposition (ALD) enables the direct, visible PEC water oxidation on solution-processed organic semiconductor thin films with enhanced stability and performance. N-type fullerene-derivative thin films passivated by sub-2 nm ALD ZnO allowed the visible PEC water oxidation at wavelengths longer than 600 nm in harsh alkaline electrolyte environments with up to 30 μA/cm² photocurrents at the thermodynamic water-oxidation equilibrium potential, which is accompanied by the photoanode half-lifetime extended to ~1000 s. The investigation shows that the enhanced water oxidation catalytic activity is afforded by the ALD ZnO passivation, and the hole transfer through the passivation layer governs the charge collection process. Further improved PEC water splitting performances were realized by improving the bottom ohmic contact to the organic semiconductor, again via the ZnO interlayer implemented by ALD, ultimately achieving ~60 μA/cm² water oxidation photocurrent at the equilibrium potential, the highest value reported for organic semiconductor thin films to our knowledge. The results not only highlight

the significant utility of ALD on improving the stability and performance of organic-semiconductor-based solar water splitting but also provide important design guidelines for optimal ultrathin passivation on organic semiconductor photoelectrodes.

AA1-TuP-15 Enhancement of Photovoltaic Efficiency using a Novel Nickel-4 Mercaptophenol Hybrid Interfacial Layer, S Mo, Jinseon Park, N Long, H Thu, Hanyang University, Republic of Korea

In this work, we introduced a novel Ni-4 mercaptophenol (Ni4MP) as an interfacial layer in Sb₂S₃-sensitized mesoporous TiO₂ solar cells. Ni4MP thin films with controllable thickness were prepared by an integrated approach via atomic/molecular layer deposition techniques and were systematically characterized. Introduction of the Ni4MP interlayer significantly enhanced the photovoltaic performance and the interfacial charge transfer kinetics of Sb₂S₃-sensitized solar cells. The augmentation of open circuit voltage and short circuit density due to the insertion of a Ni4MP interlayer enhanced the power conversion efficiency of the solar cells from 2.07% to 2.79%, corresponding to a 35% increase in efficiency. This improvement in device performance was discussed based on the energy band diagram. We found that the Ni4MP interlayer can effectively extract the photo-generated holes from the Sb₂S₃ sensitizer due to the excellent band matching and hole scavenging characteristics, thus enhancing the charge transport and suppressing the recombination.

AA1-TuP-16 Enhancement of Photovoltaic Properties of Metal/III-V Schottky Solar Cells using Al₂O₃ Anti-Reflection and Passivation Layer, A Ghods, V Saravade, C Zhou, Ian Ferguson, Missouri University of Science and Technology

The metal-semiconductor (M-S) Schottky junction structure is gaining traction in photovoltaic device applications compared to *p-n* junction structure, due to simplicity in device processing, possibility of development of high efficiency multi-junction structures, and also cost-effective large-scale device fabrication¹. III-V compound semiconductors with direct bandgap and short absorption depth are suitable candidates for fabrication of high efficiency solar cells. Schottky solar cells based on Au/Al_{0.3}Ga_{0.7}As/GaAs heterostructure have been designed and fabricated, resulting into short-circuit current density and power conversion efficiency of 20.46 mA/cm² and 4.84%, accordingly².

One of the main issues regarding the M-S structures for solar cells remains about the high reflectivity from the top metal surface. This leads to significant reduction in photon absorption in the active layer of solar cell and, therefore, lowered photo-generated current. Graphene and indium-tin-oxide (ITO), with transmission of more than 80% in the visible region, have been used in conjunction with *n*-GaAs to create Schottky solar cells, leading to short circuit current density and power conversion efficiency of up to 19 mA/cm² and 11.1%, respectively^{3,4}.

Anti-reflection coating (ARC), such as aluminum oxide (Al₂O₃), has been used to reduce the reflection from top surface of M-S Schottky solar cells, and enhance the photovoltaic properties of these devices. In this work, an 80 nm Al₂O₃ has been grown on the whole top surface of the Ag/*n*-GaAs Schottky solar cell using atomic layer deposition (ALD) technique at 200°C, Figure 1 (attachment). The initial optical measurements show the reduction of reflection from the solar cells from 48% (without ARC) to 16% (with ARC), indicating the improvement in photon absorption, Figure 2. *J-V* and EQE measurements will be performed to extract the photovoltaic properties of these devices and investigate the effect of ARC on M-S structure.

Moreover, the effect of Al₂O₃ as passivation layer will be studied in the full paper. Initial measurements have indicated a decrease in leakage current between the metal contacts, leading to enhancement of shunt resistance from 3×10⁴ W to 1×10⁵ W. This will be further investigated, and changes in photovoltaic properties of the solar cells, including filling factor, reverse saturation current, and power conversion efficiency, will be reported.

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AA1-TuP-17 Investigation of ALD-grown i-ZnO Buffer Layer Properties for CIGS Solar Cell Application, Jeha Kim, V Arepalli, Cheongju University, Republic of Korea; W Lee, Y Chung, Electronics and Telecommunications Research Institute, Republic of Korea

Zinc oxide (ZnO) is a wide bandgap (3.4 eV) *n*-type semiconductor material that can be mostly used in various optoelectronic applications from thin

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film transistors (TFTs) to solar cells due to its excellent optical and electrical properties [1]. In the CIGS solar cell device structure, the i-ZnO thin film acts as a buffer layer that reduces the leakage of shunt current paths and also it improves p-n hetero-junction quality. In the present study, we deposited the i-ZnO thin films from 80°C to 180°C onto both Si (100) and soda lime glass (SLG) by using atomic layer deposition (ALD) method. The as-grown films were characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), X-ray diffraction, UV-Vis-NIR spectroscopy, and Hall effect measurements. The thickness of as-grown ZnO films is independent of the growth temperatures from 100°C to 180°C. All samples exhibit the optimal bandgap of 3.24 eV. The ZnO buffers show the electrical resistivity of $6 \Omega \times \text{cm}$, $0.29 \Omega \times \text{cm}$, and $0.0058 \Omega \times \text{cm}$ for the films-grown at 80°C, 100°C, and 150°C, respectively. In addition, we investigated the J-V characteristics of the fabricated CIGS solar cells using ALD-grown i-ZnO buffers prepared at 80°C, 100°C, and 150°C. The solar cell fabricated with i-ZnO buffer grown at 100°C exhibits the best power conversion efficiency (η) of 8.59% with V_{oc} of 470 mV, J_{sc} of 28.84 mA/cm², and FF of 63.48%.

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AA1-TuP-18 Atomic Layer Deposited Zirconium-doped ZnO Transparent Conductive Oxides for Silicon Solar Cells, Geedhika Kallidil Poduval, M Hossain, B Hoex, University of New South Wales, Australia

Transparent conductive oxides (TCOs) are intensively investigated due to their ability to conduct charge carriers and transparency in the visible light in various fields ranging from large scale displays to photovoltaic devices. Currently, the most widely used TCO is indium tin oxide (ITO) which simultaneously offers high optical transparency and high electrical conductivity. Limited reserves, increasing indium prices, and free carrier absorption due to relative high carrier concentration have been the motivation to explore other TCO materials. Some of the alternatives to ITO are, doped ZnO, SnO₂, Cu₂O, and TiO₂.

Among the various kinds of silicon solar cell architectures, heterojunction (HET) silicon solar cells consisting of crystalline silicon absorber and amorphous silicon (a-Si) surface passivation and doped a-Si as the electron and hole selective layers implement TCOs to improve the lateral conductivity of collected carriers. As a-Si degrades at temperatures >200°C and sputtering of ITO damages the interface, leading to increased absorption and recombination, a surface sensitive low-temperature self-limiting process such as atomic layer deposition is very appealing.

In this work, Zr is used as a dopant to increase the mobility and reduce parasitic absorption of earth-abundant ZnO. The recipe for ZrO₂ growth using Tetrakis(dimethylamido) zirconium(IV) (TDMAZ) was developed and optimized on a Fiji G2 plasma enhanced ALD tool. The growth properties were studied by *in-situ* spectroscopic ellipsometry. The effects of doping (0-29 at.% Zr) were investigated for 40 nm thick films. ZnO and ZrO₂ supercycles at different ratios were carried out, and their influence on optical and electrical properties was investigated. A slight increase in mobility of ~5% up to $19 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ was observed by doping ZnO with 2.4% Zr, and the mobility reduces with increased doping. The optical band gap of ZnO increases with doping level up to a value of 3.42 eV at 10% Zr and reduces for higher Zr concentrations. First-principles density functional theory (DFT) calculations reveal the formation of defects states in the conduction band resulting from the substitutional replacement of Zn by Zr. XPS results indicate that the Zr ions in ZnO are in the Zr⁺⁴ oxidation state thereby contributing two additional electrons to the lattice. This results in an increase in carrier concentration from $2 \times 10^{19} \text{ cm}^{-3}$ to $1.2 \times 10^{20} \text{ cm}^{-3}$. Elemental depth profiling using ToF-SIMS is currently ongoing and will be shown at the time of the conference. The improvement in TCO properties of ZnO upon doping with Zr opens the possibility for applications in silicon solar cells as well as thin film solar cells.

AA1-TuP-19 Atomic Layer Deposition of Few-Atom Cluster Arrays for Solar Fuel Catalysis, David Mandia, N Gusinger, A Martinson, Argonne National Laboratory

Solar fuels catalysis is vital to developing new technologies for creating value-added products from alternative feedstocks, such as carbon dioxide and water. Inhomogeneities in typical "state-of-the-art" synthesis techniques for heterogeneous catalysts severely limit the accuracy of determining the chemical composition of active sites and elucidating mechanistic details for catalysis. In the present work, we synthesize discrete, few-atom metal oxide cluster arrays to gain insight into the relationship between cluster size/shape and catalytic activity/efficiency. Clusters are synthesized with exquisite synthetic control via atomic layer deposition (ALD) on chemically modified epitaxial graphene (EG) on SiC. Metal oxide/nitride/sulfide ALD thin film growth is strongly inhibited on graphene. Understanding the factors contributing to unintentional and intentional nucleation and growth on EG will benefit from the use of an accurate, precise imaging technique such as STM. Furthermore, we employ an *in-situ* plasma treatment (H₂, N₂, O₂) of EG to create attachment points for intentional cluster nucleation via ALD. Discrete, few-atom clusters will be synthesized and cluster size, morphology, distribution, and density of states will be determined via STM/XPS/AFM/Raman mapping. We will correlate these parameters to catalytic activity and efficiency for solar fuels catalysis.

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