ALD Applications
Room Plaza ABC - Session AA-MoM

Solar Materials I (8:00-10:00 am)/Solar Materials II (10:45 am-12:00 pm)

Moderators: Christian Dussarrat, Air Liquide, Mariadriana Creatore, Eindhoven University of Technology, The Netherlands, Jeffrey Elam, Argonne National Laboratory, Neil Dasgupta, University of Michigan

8:00am AA-MoM-1 Atomic Layer Deposition Processing for Perovskite Solar Cells: Research Status, Opportunities and Challenges, *Mariadriana Creatore,* Eindhoven University of Technology, Netherlands   **INVITED**
Organo-metal halide perovskite solar cells have exhibited a sky-rocketing conversion efficiency above 20% in just a few years. In this contribution I will address the opportunities which ALD offers to perovskite solar cells [1] by highlighting its merits of delivering high quality thin metal oxides [2], engineering the charge transport layer/perovskite interfaces [2] and being compatible with low-temperature processing (directly on the perovskite absorber) [3].

Specifically, I will address the following case studies:

· Plasma-assisted ALD TiO_2 (cycles consisting of $Ti(Cp^{Me})(NMe_2)_3$ and O_2 plasma exposure steps) is adopted in $MeNH_3PbI_3$ perovskite solar cells [2], with the purpose of suppressing charge recombination processes at the ITO/perovskite absorber/hole transport layer interface. The superior performance of 10 nm thick ALD TiO_2 layers (up to 16% cell efficiency under $1000/m^2$ illumination and 24% under indoor illumination) with respect to conventionally adopted spray pyrolysis TiO_2 correlates with the lower reverse dark current measured for ALD TiO_2, i.e. its superior blocking character toward charge recombination.

· Plasma-assisted ALD SnO_2 (cycles consisting of $Sn(NMe_2)_4$ and O_2 plasma exposure steps) is adopted as electron transport layer in a n-i-p $Cs_x(MA_yFA_{1-y})_{1-x}Pb(I_z,Br_{1-z})_3$ solar cell. The cell efficiency reaches the value of 15.9±0.5%, while the same solar cell configuration with an electron-beam deposited TiO_2 electron transport layer reaches an efficiency of just 10 ±0.5%.

· Ultra-thin (10-15 ALD cycles) Al_2O_3 is conformally deposited at 100°C by thermal ALD on a $MAPbI_{3-x}Cl_x$ perovskite layer in a n-i-p configuration [3]. The cell exhibits superior device performance with a stabilized PCE of 18%, a significant reduction in hysteresis loss and enhanced long-term stability (beyond 60 days) as a function of the storage time in ambient air, with humidity conditions of 40-70% at room temperature.

This contribution will end by discussing the challenges yet to be met by ALD processing directly on the perovskite absorber [1], in a process window requiring either higher substrate temperature or the application of plasma (as in the case of replacement of organic charge transport layers with ALD metal oxides MoO_x and NiO). In all these cases, a careful interface engineering needs to include several aspects potentially affecting the stability of the active components of the perovskite solar cell.

[1] V. Zardetto et al., Sustainable Energy and Fuels, DOI: 10.1039/c6se00076b (2017)

[2] F. Di Giacomo et al., Nano Energy 30, 460 (2016)

[3] D. Koushik et al., Energy and Environmental Science, 10, 91 (2016)

8:30am AA-MoM-3 Atomic Layer Deposition of NbC-Al2O3 Nanocomposite Films for Efficient Solar Selective Coatings, *Jason Avila,* Argonne National Laboratory*; A Peters,* Northwestern University*; A Mane, J Libera, A Yanguas-Gil,* Argonne National Laboratory*; O Farha, J Hupp,* Northwestern University*; J Elam,* Argonne National Laboratory, USA
Solar selective films hold great promise for improving the efficiency of concentrated solar power (CSP) facilities. In this study, we used atomic layer deposition (ALD) to prepare solar selective films composed of metal-dielectric nanocomposites with tunable optical and electronic properties. We used niobium carbide (NbC) as the metallic component and Al_2O_3 as the dielectric component of the nanocomposite films, and these components were blended at the atomic scale by alternating between the NbC and Al_2O_3 ALD processes. In-situ quadrupole mass spectrometry and quartz crystal microbalance (QCM) measurements were performed to examine the growth of the NbC-AlO composite films as well as to establish the NbC ALD growth mechanism. These measurements revealed that the NbC inhibited the Al_2O_3 ALD, while the Al_2O_3 enhanced the NbC ALD. Next, NbC-AlO nanocomposite films wereprepared over the full range of 0-100% NbC in Al_2O_3 and the physical, optical and electrical properties were measured.

We discovered that the band gap and electrical resistivity could be precisely tuned by controlling the composition, and that higher NbC contents yielded a lower band gap and a smaller resistivity. Based on the absorption spectra of the NbC-AlO composite films, we established that 10-20% NbC yield the highest selective absorption efficiencies due their high visible light absorption and low infrared absorption. However, the selective absorption properties of the NbC-AlO composite films were lost upon annealing to 400°C in air as a result of oxidation of the NbC. Our study demonstrates the efficacy for ALD preparing metal-dielectric nanocomposite films with tunable properties to achieve a high selective absorber efficiency. By applying this technique to more thermally robust metallic materials we hope to produce solar selective coatings suitable for deployment in CSP facilities.

8:45am AA-MoM-4 Refractory Solar Selective Nanocomposite Coatings for Concentrated Solar Power Receivers, *Jeffrey Elam, A Mane, J Avila, A Yanguas-Gil, J Libera,* Argonne National Laboratory*; J Hupp, J Liu,* Northwestern University*; U Sampathkumaran, K Yu,* InnoSense LLC*; R Buck, F Sutter,* German Aerospace Center - DLR
We are developing a new strategy for fabricating high-performance selective absorber coatings for concentrated solar power receivers. These coatings are engineered at multiple length scales (Figure 1). In the 0.1-1 μm regime, the coatings have a photonic crystal structure composed of a periodic mesoporous array. This structure alters the photonic density of states to improve spectral selectivity while also mitigating thermal stress for improved lifetime. At the 1-10 nm scale, the coatings are composed of optically absorbing nanoparticles in a transparent matrix where the size, spacing, and composition of the nanoparticles are tailored to tune the optical properties for high visible absorption and low IR emittance - similar to a cermet, but with greater thermal stability. The mesoporous photonic structure is fabricated by self-assembly from a nanoparticle suspension to form a porous matrix. The nanophase composite is created by infiltrating this scaffold using atomic layer deposition (ALD) films composed of metallic and dielectric components. We are evaluating a range of processing methods for the mesoporos scaffold and targeting sturctures guided by finite difference time domain (FDTD) modeling. In addition, we have undertaken a design of experiments (DOE) study of ALD nanocomposite films to establish the effects of composition, metal:dielectric ratio, and thickness on the optical efficiency. These studies have yielded simple design rules to predict the optical properties of the solar selective coatings, allowing us to focus on optimizing the high temperature stability and manufacturability of the materials. We have identified coatings that maintain a high selective solar absorption efficiency of $\eta_{sel} > 0.91$ after isothermal treatment and temperature cycling at 650°C with no delamination. This presentation will focus on the growth and optical properties of the ALD nanocomposites.

9:00am AA-MoM-5 P-type Bismuth Sulfide (Bi_2S_3) Grown by Atomic Layer Deposition, *Neha Mahuli, D Saha, S Sarkar,* Indian Institute of Technology Bombay, India
Bismuth sulfide (BiS_3) thin films are investigated with a custom built laminar flow atomic layer deposition system. Sequential exposures of bismuth(III)bis(2,2,6,6-tetramethylheptane-3,5-dionate) [$Bi(thd)_3$] and hydrogen sulfide (H_2S) are optimized at 200°C via various *in-situ* and *ex-situ* characterizations. Detailed growth mechanism study with the help of *in-situ* quartz crystal microbalance (QCM) and *ex-situ* X-ray reflectivity (XRR) measurements indicated the film growth governs reasonably longer nucleation periods before entering into linear ALD regime. The saturated growth rate of 0.34-0.37Å per ALD cycle is observed throughout ALD temperature window of 200-250°C.

During this presentation apart from growth mechanism, I will majorly discuss the structural, optical and electrical properties of the as-grown material. Interestingly this material is observed to exhibit presence of direct (1.45 eV) as well as indirect (1.2 eV) band gaps. A relatively high absorption coefficient (> 10^6 cm^{-1}) throughout the visible range makes it a potential photovoltaic absorber.

Contradictory to the conventionally observed, as-grown thin films are found to be highly *p*-type conducting with carrier concentration of ca. 6.8 x 10^{18} cm^{-3} at room temperature. Seebeck measurements and ultraviolet spectroscopy (UPS) also support the *p*-type nature of as-grown films as opposed to *n*-type nature normally found in literature. In the last part of my presentation, I will discuss in detail the MIT transition as studied from temperature dependent electrical resistivity measurement in detail to understand the transport mechanism.

9:15am AA-MoM-6 Role of Fixed Charge in the Modification of Schottky Barrier Height of Metal Insulator Semiconductor Tunnel Structures, *Roderick Marstell, N Strandwitz,* Lehigh University

Electronic properties of oxide/semiconductor interfaces are important in most semiconductor applications. The effectiveness of an oxide in a given application is dependent on the quality of the electronic properties of the interface, such as fixed charge (N_f), density of interface traps (D_{it}), and Schottky barrier height (ϕ_{bh}). In this study, we investigate the ability of the N_f at the oxide/Si interface to modify ϕ_{bh} of a metal-insulator-semiconductor (MIS) diode. Tunable N_f is available through atomic layer deposited (ALD) Al_2O_3, in which the N_f can be tuned from +1E12 to -5e12 q/cm^2 via post-deposition annealing.[1,2] This tunable N_f has been shown to exist in oxides as thin as 1.5 nm using non-contact techniques (corona charging and second harmonic generation).[3,4] To our knowledge, the ϕ_{bh} of a MIS diode has not been experimentally related to the magnitude of oxide/semiconductor N_f.

According to device physics simulations and analytical calculations[5], the difference in N_f in the as-deposited/annealed states should modify the ϕ_{bh} of a silicon MIS diode by as much as 100 meV. We have confirmed the presence of a negative N_f by analyzing the capacitance-voltage behavior of identical MIS stacks with insulating Al_2O_3 layers (~10 nm). Fixed charge values changed from +1E12 to -3E12 q/cm^2 depending on processing.

We measured the ϕ_{bh} of MIS diodes as a function of oxide thickness from current-voltage-temperature (*IVT*) and Mott-Schottky ($1/C^2$-V) data for oxides in the 1-2 nm range and for intimate metal/Si contact. A large change in ϕ_{bh} between the intimate contact and MIS case was found. The *IVT* data shows a decrease in ϕ_{bh} with increasing oxide thickness for both as-deposited and annealed samples, while $1/C^2$-V data does not display a ϕ_{bh} versus N_f trend. Both *IVT* and $1/C^2$-V trends are inconsistent with the electrostatic models.

Our data does not give evidence that the tunable N_f in Al_2O_3-Si MIS diodes controls ϕ_{bh}. This may indicate that the N_f affects ϕ_{bh} negligibly or not at all. Metal deposition may introduce electronic traps at the metal/oxide interface that alter the oxide/Si interface N_f. Finally, the first few cycles of ALD growth may introduce oxide thickness and/or N_f lateral non-uniformities, thus obfuscating the N_f/ϕ_{bh} relationship. While this work shows an influence of the ALD tunnel oxide layer, evidence of N_f controlling ϕ_{bh} was not found.

1. J. Frascaroli et al, Phys. Stat. Solidi A-Appl. Mat. **210,**4732-736(2013)

2. G. Dingemans et al, Electrochem. And Solid-State Let. **14,**1H1(2011)

3. G. Dingemans et al, J. Appl. Phys. **110,**093715-1(2011)

4. F. Werner et al, J. Appl. Phys. **109,**11113701(2011)

5. R. T. Tung, Appl. Phys. Rev. **1,**1011304(2014)

9:30am AA-MoM-7 Determination of Energy Barrier Heights between Amorphous Metals and ALD Dielectrics using Internal Photoemission Spectroscopy, *Melanie Jenkins, T Klarr, D Austin, J McGlone,* Oregon State University*; L Wei, N Nguyen,* National Institute of Standards and Technology*; J Wager, J Conley,* Oregon State University

High quality ALD insulators are an enabling technology for thin film metal-insulator-metal (MIM) tunnel diodes.[1] High speed MIM diodes show promise for rectenna based energy harvesting of IR radiation, for IR sensing, and as building blocks for beyond CMOS hot-electron (MIMIM) transistors. Operation of these devices is based ideally on Fowler-Nordheim tunneling, which is exponentially dependent on both the thickness of the insulator and the height of the energy barriers between the metal electrodes and the insulator. Accordingly, smooth bottom electrodes and precise knowledge of metal/insulator barrier heights are critical for predicting, understanding, and optimizing MIM diode device operation. Although insulator thickness can be precisely controlled through ALD, actual barrier heights depend strongly on deposition method as well the exact interface, and typically differ significantly from the simple Schottky-Mott rule. In this work, we use internal photoemission (IPE) spectroscopy to measure and compare the barrier heights between two ultra-smooth amorphous metals (ZrCuAlNi and TaWSi) and several ALD insulators in MIM diode structures. Reports of IPE on MIM structures are relatively uncommon.

MIM diodes consist of either a ZCAN or TaWSi bottom electrode deposited onto 100 nm of SiO_2 on Si. (ZCAN has been shown to function well in MIM diodes,[2] but suffers from thermal instability. TaWSi is a new amorphous metal that has a larger work function than ZCAN and improved thermal stability.) 10-20 nm of Al_2O_3, HfO_2, and ZrO_2 were then deposited via ALD using TMA/H_2O at 300°C, and TEMA-Hf or TEMA-Zr / H_2O at 250°C,

respectively. SiO_2 was deposited via PEALD using $BDEA$-Si/O_2 at 200 °C. Semitransparent (10 nm thick) Al or Au top electrodes were evaporated through a shadow mask.

IPE measurements were performed at both NIST and OSU. Voltage was applied to the bottom electrode and current was measured while photon energy (E_{ph}) was swept from 2 to 5 eV. The measured current was corrected to remove dark current and converted to yield. Voltage dependent spectral thresholds were extracted from plots of the square root of yield vs. E_{ph}. Zero-field barrier heights were obtained from Schottky plots of the spectral thresholds vs. square root of the dielectric field (Fig 1). The TaWSi electrodes show consistently higher barrier heights than the ZCAN electrodes (Fig. 2), indicating promise for application as a thermally stable bottom electrode in MIM tunnel diodes.

[1] N. Alimardani et al., J. Appl. Phys. 116, 024508 (2014).

[2] N. Alimardani et al., J. Vac. Sci. Technol., A 30(1), 01A113 (2012).

9:45am AA-MoM-8 ALD Window and Buffer Layers in Thin Film Solar Cells, *A Palmstrom, K Bush, M McGehee, A Hultqvist, T Sone, **Stacey F. Bent**,* Stanford University

Modern solar cells contain stacks of different semiconducting, insulating and conducting materials with optoelectronic properties that need to be tightly controlled. Atomic layer deposition (ALD) is poised to play a role in generating various component materials for solar cells with a high level of control over composition, structure, and thickness. ALD has already been used to deposit passivation layers, buffer layers, barrier layers, and even in the case of plasmonic solar cells, absorber layers. We will present results on the application of ALD to the buffer layer of $Cu(In,Ga)Se_2$ (CIGS) cells and to the window layer in hybrid lead halide perovskite solar cells. CIGS thin-film technology provides efficiencies close to those of conventional Si based cells. However, the cells typically contain CdS buffer layers, and alternative, less-toxic buffer layers have not performed as well due to charge recombination at the buffer layer/CIGS interface. We introduce a device design that utilizes a point contact buffer layer, for which fabrication is carried out by a combination of ALD and nanosphere lithography. We demonstrate proof of concept using Al_2O_3 as the passivating material, ZnO as the conductive material, and a silica nanosphere size of ~300 nm in diameter. The resulting point contact CIGS solar cells yield a higher conversion efficiency (6.58 ± 0.58%) than either of the binary buffer layers Al_2O_3 (0%) and ZnO (5.15 ± 0.57%). The improvement over ZnO is attributed to an increased open circuit voltage, which is an indication of a reduced surface recombination. Hybrid lead halide perovskites are promising candidates for low cost, thin film light absorbers; they have a tunable band gap and have demonstrated efficiencies as high as 22.1%. The perovskites are also of interest for wide-bandgap absorbers in tandem photovoltaics. We investigate the use of a bilayer consisting of a semiconductor, tin oxide, and a transparent conducting oxide, zinc tin oxide, deposited on top of perovskite absorbers by ALD as a dual-purpose layer to achieve electron selectivity and sputter protection with high optical transmission. This bilayer is applied to two tandem systems: perovskite-perovskite and perovskite-silicon devices. We demonstrate perovskite-perovskite efficiencies of 17.0% with a monolithic two-terminal tandem and 20.3% with a mechanically-stacked four-terminal cell. We achieve an NREL-certified 23.6% efficiency in a perovskite-silicon monolithic tandem architecture. Furthermore, we show that the perovskite encapsulation, enabled by ALD, results in impressive cell stability by testing for 1000 hrs with less than 10% degradation in performance.

10:45am AA-MoM-12 Atomic Layer Deposition of Bismuth Vanadate Photoanodes, *Ashley Bielinski, J Brancho, B Bartlett, N Dasgupta,* University of Michigan, USA

Artificial Photosynthesis is a promising route for capturing solar energy and storing it in the form chemical bonds to generate useful fuels. For example, solar-driven water splitting to produce H_2 and O_2 is widely viewed as an enabling technology for solar-to-fuel conversion. Many Photoelectrochemical (PEC) cells are limited by low anodic currents, due to tradeoffs between light absorption, carrier separation, and interfacial stability in aqueous electrolytes. A good photoanode must be an n-type semiconductor that absorbs in the visible spectrum and has a valence band that is more positive than the oxygen evolution potential. Bismuth vanadate (BVO) has been demonstrated as one of the most promising visible light absorbing photoanode materials. With a bandgap of 2.4V and favorable band positions, BVO has the potential to achieve high anodic

photocurrents. However, BVO suffers from limited electron-hole separation, charge transport, and water oxidation kinetics.

Nanostructured BVO, and particularly core-shell nanowires address these challenges by decoupling the required absorption carrier diffusion lengths.[1] Core-shell heterojunctions can also aid in charge separation and transport. Atomic layer deposition (ALD) is an ideal technique for the conformal coating of complex nanostructures. The development of ALD BVO enables core-shell nanostructured BVO photoanodes with much greater conformal coverage and thickness control than previously demonstrated solution deposition methods.

Herein, we demonstrate ALD of BVO using $Bi(OCMe_2iPr)_3$ as the bismuth source, vanadium(V) oxytriisopropoxide as the vanadium source, and water as the oxidant. This combination of precursors enables full control of the Bi:V ratio, in contrast to the use of bismuth precursors such as $Bi(thd)_3$ and triphenylbismuth, which also suffer from very low growth rates (<0.1 Å/cycle). We demonstrate the deposition of stoichiometric $BiVO_4$ and the annealing of ALD BVO to achieve the photoactive monoclinic phase. X-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), and ultraviolet–visible (UV-Vis) spectroscopy are used to study the composition, crystallographic, and optical properties of the ALD BVO. The photoactivity of the ALD BVO for the oxidation reaction was demonstrated on both planar and core-shell nanowire arrays under simulated AM 1.5G illumination, demonstrating the power of ALD to improve light absorption and charge extraction in 3-D nanostructured architectures.

(1) Liu, C.; Dasgupta, N. P.; Yang, P. *Chem. Mater.***2014**, *26* (1), 415–422.

11:00am AA-MoM-13 High-Efficiency Perovskite Solar Cells with Humidity-Stability beyond 60 Days Achieved via Atomic Layer Deposition, *Dibyashree Koushik, Y Kuang,* Eindhoven University of Technology, Netherlands*; V Zardetto,* TNO-Solliance, High Tech Campus, Netherlands*; W Verhees, S Veenstra,* ECN-Solliance, High Tech Campus, Netherlands*; M Verheijen, W Kessels, M Creatore, R Schropp,* Eindhoven University of Technology, Netherlands

Solar cells based on organic-inorganic hybrid perovskites have recently achieved an astounding power conversion efficiency (PCE) of 22.1% placing themselves at the fore-front of many of the current global photovoltaic (PV) technologies. However, in order to scale-up the perovskite PV technology, the issue regarding its device lifetime needs to be addressed, which is one of the major hurdles towards its successful commercialisation. The most conventional and widely used perovskite, the methylammonium lead iodide ($CH_3NH_3PbI_3$) is highly sensitive to oxygen and moisture due to the presence of the weak Pb-I ionic bonds and the volatile CH_3NH_3I component in its lattice structure. Several attempts have been made to address this instability issue, mostly concentrating on the substitution of the organic cations in the perovskite lattice, and on alternatives for the organic charge extraction layers, without laying much emphasis on stabilising the existing, conventional high efficiency $CH_3NH_3PbI_3$/Spiro-OMeTAD based perovskite solar cells (PSCs).

To address the latter issue, we present an atomic layer deposition (ALD) assisted interface engineering approach, which consists of incorporating an ALD Al_2O_3 layer, deposited directly on top of the $CH_3NH_3PbI_{3-\delta}Cl_\delta$ perovskite film.[1-3] This Al_2O_3 layer substantially protects the underlying sensitive perovskite against humidity,[1] and also provides protection from other cell components during their respective depositions on top of the perovskite,[3] thus preventing premature device failure. In addition, it does not preclude the formation of a low-resistance contact to the perovskite layer. The fabricated PSCs exhibit superior device performance with a PCE of 18% (with respect to 15% of the pristine), a significant reduction in the hysteresis loss, and an unprecedented long-term stability (beyond 60 days) as a function of the unencapsulated storage time in ambient air, under humidity conditions ranging from 40% to 70% at room temperature. PCE measurements after 70 days of aging study show that the devices incorporating 10 cycles of ALD Al_2O_3 retain about 60-70% of the initial PCE, while the reference devices drop to about 12% of the initial PCE.[1]

[1] D. Koushik, W. J. H. Verhees, Y. Kuang, S. Veenstra, D. Zhang, M. A. Verheijen, M. Creatore, R. E. I. Schropp, *Energy & Environmental Science* **2017**, *10*, 91.

[2] V. Zardetto, B. L. Williams, A. Perrotta, F. Di Giacomo, M. A. Verheijen, R. Andriessen, W. M. M. Kessels, M. Creatore, *Sustainable Energy & Fuels* **DOI:**10.1039/C6SE00076B

[3] D. Koushik, W. J. H. Verhees, D. Zhang, Y. Kuang, S. Veenstra, M. Creatore, R. E. I. Schropp, *Advanced Materials Interfaces* (**Accepted**).

11:15am AA-MoM-14 Efficient Surface Passivation of Black Silicon Using Spatial ALD, *I Heikkinen,* Beneq Oy, Finland*; P Repo, V Vähänissi, T Pasanen,* Aalto University, Finland*; V Malinen, **Emma Salmi,*** Beneq Oy, Finland*; H Savin,* Aalto University, Finland

Nanostructured Si surfaces (b-Si) are promising materials in photovoltaic applications, but their large area requires efficient passivation. Remarkable passivation of b-Si has been demonstrated with Al_2O_3 deposited by temporal ALD, and this result has been applied in record-breaking solar cells [1]. Spatial ALD (SALD) aims to increase the deposition rate of conformal coatings and broaden the reach of ALD. SALD is potentially well applicable in the coating of porous structures, as precursors are injected towards the substrate with high concentration, which presumably facilitates the infiltration of reactants to the bottom of the structure [2]. Few studies on coating HAR structures with SALD have been published, but there is growing interest in SALD in *e.g.* the coating of porous battery electrodes [3]. In this study we show that excellent passivation of b-Si can be achieved with SALD.

Both planar and b-Si samples were passivated using a Beneq sheet-to-sheet SALD reactor SCS 1000 with a maximum coating area of 400 mm x 500 mm. 20 nm thick Al_2O_3 layers were deposited on the substrates using TMA and H_2O as precursors at 150°C with line speeds ranging from 1.5 to 9 m/min. Growth per cycle ranged from 1.27 to 1.49 Å/c depending on the line speed, and deposition rates up to 2.9 nm/min were reached. As shown in Figure 1a, efficient passivation of planar substrates was demonstrated with all line speeds, as charge carrier lifetimes τ in the order of 1 ms were reached. Substrates were post-annealed at 370 to 450°C in N_2 and H_2/N_2 atmospheres to study the effect of the annealing conditions to τ. As seen in Figure 1b, the best lifetime for both planar and b-Si samples is obtained by annealing at 370°C in a H_2/N_2 atmosphere.

Similar planar and b-Si wafers were passivated using temporal ALD (Beneq TFS 500) and TMA and H_2O as precursors at 200°C. Previously optimized annealing at 425°C in N_2 atmosphere was chosen for these samples. The highest lifetimes of SALD-coated planar and b-Si wafers were compared with the best results obtained with temporal ALD. T as a function of minority carrier density of SALD and temporal ALD passivated wafers are presented in Figure 2. Experiments showed that SALD can provide similar or even better surface passivation in b-Si than temporal ALD. This is a promising indication that conformal coating of HAR structures such as b-Si is feasible and possibly even more efficient with SALD than with temporal ALD. Efficient passivation of b-Si substrates was achieved with an industrially relevant line speed of 1.5 m/min. As high production rates can be reached, passivating b-Si with SALD has great potential in industrial-scale applications.

11:30am AA-MoM-15 Enhancing Water Oxidation Activity of α-hematite Through Atomic Layer Deposition, *C Du, J Wang,* Huazhong University of Science and Technology, China*; R Chen,* Huazhong University of Science and Technology, China, P.R. China*; Y Wen, **Bin Shan,*** Huazhong University of Science and Technology, China

Photoelectrochemical water splitting holds great potential for solar energy conversion and storage with zero greenhouse gas emission. Among existing semiconductor absorber candidates, hematite (α-Fe_2O_3) stands out with unique combination of ideal band gap (2.0-2.1 eV), non-toxicity, earth abundance and intrinsic N-type behavior. However, its faces sever challenges of low photovotlage and conversion efficiency which greatly limit its practical application at current stage.

Because of its unique self-limiting reaction chemistry, Atomic Layer Deposition (ALD) technique exhibits prominent advantage in fabrication of heterojunctions with controllable film thickness. It plays an important role in enhancing the PEC water splitting performance, especially in the case with high aspect ratio light absorber architectures. In our study, ALD is adopted to enhance the quantum efficiency of nanostructured hematite film through two different strategies, p-n heterojunction and surface modification with co-catalyst. In the first work, *p*-$LaFeO_3$/*n*-Fe_2O_3 heterojunction is achieved by depositing La_2O_3 on *β*-FeOOH nanorod, followed by post thermal treatment at 800 °C. Due to the well matched band levels of $LaFeO_3$ and α-Fe_2O_3, the onset potential for photocurrent negatively shifted by ~50 mV in the heterojunction photoanode. In the second study, nanostructured hematite film was coated with an ultrathin CoO_x overlayer through Atomic Layer Deposition. The best performing hybrid hematite with 2-3 nm ALD CoO_x overlayer yields a remarkable turn on potential of 0.6 V_{RHE} for water oxidation reaction, with a significant 250 mV enhancement compared bare hematite electrode. Meanwhile, external quantum efficiency (IPCE) obtained on hematite increases 66% at 1.23V_{RHE}.

The unique surface amorphous CoO_x /$Co(OH)_2$ prepared by low temperature ALD exhibits good optical transparency and hydrophilic property, which is beneficial to the formation of ideal hematite/electrolyte interface.

11:45am **AA-MoM-16 ALD Stabilization Layers for Quantum Dot Solar Energy Conversion**, *Theodore Kraus, B Parkinson,* University of Wyoming

Quantum dot sensitized solar cells (QDSCs) are an emerging area of solar energy conversion research with potential to compete with current Si and thin film solar technologies. Quantum dots (QDs) are intriguing candidates for solar power conversion systems as they have large extinction coefficients and a size dependent tunable band gap allowing for utilization of much of the solar spectrum. Furthermore, upon photoexcitation QDs have shown the ability to inject photoexcited carriers from higher excited states and produce quantum yields for electron flow of greater than 1 via multiple exciton generation (MEG).[1] Despite their useful properties many quantum dot systems are unstable to oxidation under atmospheric conditions and in aqueous electrolytes. These stability issues currently present a challenge for the synthesis and characterization of certain QD systems such as InSb and PbSe QDs that are of particular interest due to their near IR band gaps and potential to exhibit MEG.

In this research metal oxide layers grown using atomic layer deposition (ALD) are investigated as stabilization layers for model QDSC interfaces. Specifically, quantum dot sensitized single crystal metal oxide substrates are prepared and subsequently coated with ALD stabilization layers. Metal oxides are chosen for these stabilization layers as they are typically inert, and have large band gaps that do not block light from reaching the QDs. In addition to these desirable properties, there are numerous of metal oxides that can be deposited using commercially available ALD precursors.[2] In addition to the wide variety of oxide materials that can be prepared using ALD, it is an ideal technique to produce ultrathin, highly conformal stabilization layers in a vacuum environment at lower temperatures compared to chemical vapor deposition. In this work we prepare model QDSC interfaces on well-characterized metal oxide single crystal substrates with thin ALD metal oxide protection layers and test their stability in air and in electrolytes under photoexcitation.

References

[1] J. B. Sambur, T. Novet, and B. A. Parkinson, " Multiple Exciton Collection in a Sensitized Photovoltaic System, " Science 330, 63 (2010)

[2] V. Miikkulainen, M. Leskela, M. Ritala, and R. L. Puurunen, "Crystallinity of inorganic films grown by atomic layer deposition: Overview and general trends," J. Appl. Phys. 113, 021301 (2013)

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— H —
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Hultqvist, A: AA-MoM-8, 2
Hupp, J: AA-MoM-3, 1; AA-MoM-4, 1
— J —
Jenkins, M: AA-MoM-7, **2**

— K —
Kessels, W: AA-MoM-13, 3
Klarr, T: AA-MoM-7, 2
Koushik, D: AA-MoM-13, **3**
Kraus, T: AA-MoM-16, **4**
Kuang, Y: AA-MoM-13, 3
— L —
Libera, J: AA-MoM-3, 1; AA-MoM-4, 1
Liu, J: AA-MoM-4, 1
— M —
Mahuli, N: AA-MoM-5, **1**
Malinen, V: AA-MoM-14, 3
Mane, A: AA-MoM-3, 1; AA-MoM-4, 1
Marstell, R: AA-MoM-6, **2**
McGehee, M: AA-MoM-8, 2
McGlone, J: AA-MoM-7, 2
— N —
Nguyen, N: AA-MoM-7, 2
— P —
Palmstrom, A: AA-MoM-8, 2
Parkinson, B: AA-MoM-16, 4
Pasanen, T: AA-MoM-14, 3
Peters, A: AA-MoM-3, 1
— R —
Repo, P: AA-MoM-14, 3
— S —
Saha, D: AA-MoM-5, 1

Salmi, E: AA-MoM-14, **3**
Sampathkumaran, U: AA-MoM-4, 1
Sarkar, S: AA-MoM-5, 1
Savin, H: AA-MoM-14, 3
Schropp, R: AA-MoM-13, 3
Shan, B: AA-MoM-15, **3**
Sone, T: AA-MoM-8, 2
Strandwitz, N: AA-MoM-6, 2
Sutter, F: AA-MoM-4, 1
— V —
Vähänissi, V: AA-MoM-14, 3
Veenstra, S: AA-MoM-13, 3
Verhees, W: AA-MoM-13, 3
Verheijen, M: AA-MoM-13, 3
— W —
Wager, J: AA-MoM-7, 2
Wang, J: AA-MoM-15, 3
Wei, L: AA-MoM-7, 2
Wen, Y: AA-MoM-15, 3
— Y —
Yanguas-Gil, A: AA-MoM-3, 1; AA-MoM-4, 1
Yu, K: AA-MoM-4, 1
— Z —
Zardetto, V: AA-MoM-13, 3