ALD Applications
Room Halla Hall - Session AA3-WeM

Other Energy Applications

Moderators: Rong Chen, Huazhong University of Science and Technology, **Hyeontag Jeon**, Hanyang University

10:45am **AA3-WeM-12 Using Area-Selective Ald for Dual Site Catalysis for Photocatalytic Water Splitting**, ***Katherine Hurst***, *Wilson McNeary,* National Renewable Energy Laboratory*; William Stinson,* Columbia University*; Shane Ardo,* University of California Irvine*; Daniel Esposito,* Columbia University **INVITED**

ALD (Atomic Layer Deposition) of thin films on catalysts can introduce a variety of functionalities in electrochemical systems, effectively altering chemical reactions and outcomes. For example, thin films can enhance the physical stability of a catalyst on a substrate, alter the surface energy through core shell design, passivate catalyst defect sites that create side reactions, among others. Here, we explore strategic deposition of thin oxide coatings by ALD to a enhance reaction selectivity of a co-catalyst system.

Photocatalytic (PEC) water splitting uses a configuration where cocatalysts drive two separate reactions; hydrogen evolution reaction (HER), and hydrogen oxidation reaction (HOR), that are coupled by an active redox mediator to shuttle charge between them. A significant efficiency loss for PEC is caused by high rates of undesired side and back reactions, which are intensified by the proximity of the neighboring oxidation and reduction sites. In this work, we use area selective ALD (AS-ALD) of oxide films to develop tunable interface layers to prevent back reactions that hinder the efficiency.

AS-ALD was used to target growth of an oxide film on one metal of planar dual-metallic-site thin film electrode system with distinct Au regions and Pt regions. Thiol molecules acted as self-assembled monolayers adsorbed on the Au surface, preventing subsequent TiO_2 ALD growth on the Pt regions. After a mild ozone-treatment to remove the thiol molecules, the bare Au surface is exposed. The TiO2 film characteristics and spatial selectivity of growth was characterized by ellipsometry and X-ray photoelectron spectroscopy (XPS). Scanning electrochemical microscopy (SECM) measured suppressed undesired HOR and redox reactions while still permitting the desired HER, verifying the effective blocking methods of the AS-ALD approach. The capability to strategically alter dual-site reaction sites closely spaced provides a promising pathway to enhancing efficiencies in PEC systems.

11:15am **AA3-WeM-14 Impact of Tetrakis(dimethylamido)tin(IV) Degradation on Atomic Layer Deposition of Tin Oxide Films and Perovskite Solar Cells**, *Shuang Qui, Augusto Amaro,* University of Victoria, Canada*; Diana Fabulyak,* Avantor, Canada*; Julien Appleby-Millette,* University of Victoria, Canada*;* ***Cassidy Conover***, Avantor, Canada*; Dongyang Zhang, Vishal Yeddu, I. Teng Cheong, Irina Paci, Makhsud Saidaminov,* University of Victoria, Canada

Tin oxide (SnOx) films synthesized by atomic layer deposition (ALD) are widely explored in a range of optoelectronic devices, including electrochemical sensors, transistors, and photovoltaics. However, the integrity of the key ALD-SnOx precursor, namely tetrakis(dimethylamido)tin (IV) (TDMASn), and its influence on the properties of the ultimate films remain unexplored. Here, a significant degradation of TDMASn into bis(dimethylamido)tin (II) via the Sn-imine complex is reported, and its impact on the corresponding films and devices is examined. It is found, surprisingly, that this degradation does not affect the growth kinetics and morphology of ALD-SnOx films. However, it notably deteriorates their electronic properties, resulting in films with twice the electrical resistance due to different oxidation mechanisms of the degradation products. Perovskite solar cells employing such films exhibit a significant loss in power conversion efficiency, primarily due to charge transport and transfer losses. These findings urge strategies to stabilize TDMASn, a critical precursor for ALD-SnOx films, or to identify alternative materials to achieve efficient and reliable devices.

11:30am **AA3-WeM-15 Ultrathin Oxygen Deficient SnOx Films as Electron Extraction Layers for Perovskite Solar Modules**, *Helen Hejin Park,* ***Joshua Sraku Adu***, Korea Research Institute of Chemical Technology (KRICT), Republic of Korea

The fabrication of high-efficiency, large-area perovskite solar cells necessitate the development of homogeneous charge extraction layers with tunable optoelectronic properties. The characteristics of SnO_x films, deposited via thermal atomic layer deposition (ALD) and plasma-enhanced ALD (PEALD), are influenced by critical parameters such as deposition temperature, precursor pulse and purge durations, extrinsic doping, and post-annealing conditions.[1-3] Despite the homogeneity and conformity of the ALD films, the device performs poorly when compared to ETL generated using colloidal nanoparticle deposition. In this report, we describe the impact of oxygen-deficient tin oxide (SnO_x) thin films as electron extracting layers in perovskite solar modules, deposited by a highly innovative plasma-modified atomic layer deposition (PMALD) tool that allows us to further tune composition, conductivity, and effective work function.Energy-filtered photoemission of electron microscopy (EF-PEEM) shows a remarkably homogeneous surface electronic landscape of the PMALD SnO_x.We examine the impact of PMALD-SnO_x in *n-i-p* device configuration, with poly(triarylamine) (PTAA) as the hole transporting layer, which leads to the improvement in perovskite module power conversion efficiency from 17.9% to 20.1%, with an active area of 23.2 cm^2.Furthermore, devices maintained 92% of their initial efficiency for 2,700 h at 85°C and 85% relative humidity and 96% for 1,000 h under continuous 1 SUN illumination with maximum power point tracking.

References

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3. H. H. Park, *Nanomaterials*, 2022, **12**, 4326.

11:45am **AA3-WeM-16 Charge Transport Layers Rafted by Atomic Layer Deposition for Large-Area Perovskite-Based Solar Modules**, ***Femi Mathew***, Institut Photovoltaïque d'Ile-de-France (IPVF), France*; Damien Coutancier,* CNRS-IPVF, France*; Getaneh Gesesse, Marion Provost, Nadia Nazi,* Institut Photovoltaïque d'Ile-de-France (IPVF), France*; Nathanaelle Schneider,* CNRS-IPVF, France

Perovskite solar cells (PSCs) have emerged as promising solar cell technology with rapidly advancing power conversion efficiency (PCE) driven by continuous research and innovation. [1,2] To achieve efficient and stable PSCs, optimal charge transport layers are paramount. Among various vacuum based fabrication techniques, the atomic layer deposition (ALD) technique is a powerful strategy to fabricate pinhole free and electrically continuous charge transport layers with precise thickness control.[3,4] Additionally, for the large-scale production of perovskite modules, the ALD technique is particularly valuable, offering conformal deposition on large-area substrates, making it viable for commercialization.[5]

In this work, we focused on the atomic layer deposition of charge transport layers for 64 cm^2 single junction semi-transparent inverted (PIN) perovskite solar modules. The device structure is built on glass substrate, fluorine-doped tin oxide (FTO) as bottom electrode, NiO_x passivated with self-assembled monolayers (SAMs) as hole transport layer (HTL), perovskite as absorber layer, C60 and SnO_2 as electron transport layer (ETL) and indium tin oxide (ITO) as top electrode. [Fig 1(a)] Among these, the NiO_x and SnO_2 layers were deposited by ALD at low temperatures to ensure compatibility with perovskite absorber material.

Both NiO_x and SnO_2 layers deposited by ALD have been thoroughly investigated for their physicochemical and optoelectronic properties to evaluate their qualification for efficient charge extraction. The crystallinity, surface morphology and chemical composition of the NiO_x and SnO_2 films were investigated. [Fig 2(b&c)] Additionally, optoelectronic properties of the NiO_x and SnO_2 films including transmittance, bandgap and work function were also evaluated. Finally, the solar cell parameters of the device were measured and the champion device obtained PEC of 11% on large area (64 cm^2) perovskite modules. In summary, this work highlights the potential of ALD technique in the fabrication of promising charge-transport layers for next generation photovoltaic cells.

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