Electronic Materials and Photonics
Room 207 A W - Session EM2+AP+QS+TF-TuM

Evolution of Materials and Devices for Energy Harvesting and Conversion

Moderators: Seth King, University of Wisconsin - La Crosse, **Parag Banerjee**, University of Central Florida

11:00am **EM2+AP+QS+TF-TuM-13 Structural and Electronic Properties of CdSexTe1-x /CdTe thin-film photovoltaic devices: Carrier Dynamics Analysis by Charge Carrier Collection Efficiency*, Philip (Sanghyun) Lee,*** University of Kentucky*; Kent Price,* Morehead State University

Polycrystalline Cadmium Telluride (CdTe) thin-film solar cells are among the most successful commercial thin-film solar technologies, achieving a record cell efficiency of nearly 23.1% and offering competitive module costs compared to silicon (Si) modules. More than 20 GW of CdTe modules have been installed worldwide. Laboratory-scale tests have even surpassed 23.1%, getting closer to the theoretical Shockley-Queisser limit of about 32%. Recent research has focused on integrating selenium (Se) into CdTe absorbers to create band grading without the use of CdS window layers. The compound CdSexTe1-x has emerged as a key candidate for enhancing the short-circuit current (Jsc) by lowering the bandgap below 1.45 eV, which could help push short-circuit-current (Jsc) closer to its theoretical limits.

In this study, we fabricated $CdSe_xTe_{1-x}$/CdTe devices with vapor transport technology (VTD) and characterized the structural chemistry and electronic properties of $CdSe_xTe_{1-x}$/CdTe devices from the carrier collection dynamics perspective. The device structure is CdSeTe/CdTe absorbers on TEC-10 glass coated with fluorine-doped tin oxide (SnO_2:F), and finished with Gold back metal contact to minimize the impact of unwanted back contact Schottky barrier on carrier dynamics. The devices were treated under $ClCl_2$ ambient at 480 C for grain recrystallization and grain boundary passivation. Selenium (Se) diffuses deeper into the CdTe film to form CdSeTe. The device was then assessed using cross-section using Scanning Transmission Electron Microscopy (STEM) coupled with Energy dispersive X-ray analysis (STEM-EDX) in addition to evaluating device performance and characteristics. The carrier collection is measured by quantum carrier collection efficiency. The results indicate that Se uniformly diffused into CdTe grains, forming CdSeTe, which effectively lowers the bandgap energy to 1.41 eV, which is 40 mV lower than our initial calculation (1.45 eV), which increased photocurrent to 28.66 mA/cm^2. The Se concentration is approximately 5-7 %, incorporated into the front interface of $CdSe_xTe_{1-x}$/CdTe films. From the carrier dynamics analysis, the total loss of charge carrier collection is 19.6%, as compared to ideal charge carrier collection at the front heterojunction of $CdSe_xTe_{1-x}$/CdTe. This indicates that there is room to further improve charge carrier collection to achieve higher photocurrent and, thus, efficiency. The UV and violet light charge collection is 5.46 mA/cm^2, whereas the red light charge collection is 4.37 mA/cm^2. The most charge collection occurs at in-between wavelengths as 18.71 mA/cm^2.

11:15am **EM2+AP+QS+TF-TuM-14 Analysis of $KNbo_3$ Crystal Structure Fabricated on $LiNbO_3$ and $LiTaO_3$ Substrate for Piezoelectric Sensors and Devices Applications*, LAY THITHI,*** *Asuki Hagiwara, Ryotsuke Arai,* Josai University, Japan

Recently, small scales energy harvester with clean energy sources are in demand for various portable sensors and electronics devices [1]. Piezoelectric materials such as $KNbO_3$ are in focus for new type of sensors and electronic materials due to its high piezoelectric properties, high curie temperature around 450℃ as well as lead free for environmental hazard compared to lead zirconate titanate PZT [2-3]. On the other hand, piezoelectric crystal such as lithium niobate ($LiNbO_3$) and lithium tantalate ($LiTaO_3$) also have been widely used in electronic and communication devices because it has high electro-optical properties as well as high curie temperature which is considered as the most important parameter for device performance [4]. In this study, well-ordered $KNbO_3$film were synthesis on $LiNbO_3$,$LiTaO_3$ single crystals substrate by hydrothermal method aiming for possibility of electro-optical switching devices, energy conversion and other sensing devices.

$KNbO_3$ (100) and (111) structure epitaxially grown on $LiNbO_3$ and $LiTaO_3$ single crystal substrate with various reaction time and conditions. Crystal structure and film thickness were analyzed by SEM and XRD. Grains size ranging from 1-7μm and polycrystalline crystal film with thickness varies 3-10μm were obtained by single reaction. Two different substrates showed different surface morphology and crystal structure to understand lattice matching $KNbO_3$ film synthesis on $LiNbO_3$ and $LiTaO_3$ which is important for piezo electric properties [5].

[1] T. Stevenson, D. G. Martin, P.I. Cowin, A. Blumfield, A. J. Bell, T. P. Domyn, P. M. Wearver, Piezoelectric materials for high temperatures transducers and actuators, J. Matter. Scpi. Mater Electron 26, 9256-9267, 2015.

[2] Ryo Kudo, Peter Bornnann, Tobias Hemsel and Takeshi Morita, Thick KNbO3 film deposited by ultrasonic-assisted hydrothermal method, acoust. Sci. & Tech. 36, 3262-264, 2015.

[3] T. Stevenson, D. G. Martin, P.I. Cowin, A. Blumfield, A. J. Bell, T. P. Domyn, P. M. Wearver, Piezoelectric materials for high temperatures transducers and actuators, J. Matter. Scpi. Mater Electron 26, 9256-9267, 2015.

[4] M. Demartom Maeder, D. Damjanovic and N. Setter, Lead free piezoelectric materials, J. of Electro ceramics, 12, 385-392, 2004.

[5] Xiaoyan Liu, Kazuya Terabe and Kenji Kitamura, Stability of engineered domains in ferroelectric LiNbO3, LiTaO3, crystals, Phys. Scr. T129, 103-107, 2007.

11:30am **EM2+AP+QS+TF-TuM-15 Modelling the Surface Electronic Properties of Catalytic Condenser for Programmable Reactions*, Lars Grabow,*** *Shengguang Wang,* University of Houston*; Kaida Liu, Ulrick Gaillard,* University of Minnesota*; Rohit Punyapu, Rachel Getman,* Ohio State University*; Matthew Neurock,* University of Minnesota **INVITED**

The evolution of catalyst design has progressed from structural control and optimization to dynamic electronic control of active sites for surface chemistry. This advancement enables precise tuning of active sites via potential, light, or strain applied to material surfaces. Catalytic condensers are novel devices that stabilize charge from an applied potential across a high-κ dielectric film in a thin top layer of carbon with active sites on metal nanoclusters. This talk examines several computational methods to calculate charge condensation on catalytic condensers and the influence on the adsorption of atomic and molecular species.

The tested methods include direct quantum chemical cluster calculations, charged periodic calculations with homogeneous background counter charge, implicit solvation methods, localized countercharge within the vacuum region, and explicit charge transfer atoms within the vacuum region. Density functional theory (DFT) calculations were employed to evaluate these methods, providing insights into the influence of condensed charge on adsorption and assessing the accuracy and computational requirements of each approach.

The study systematically varied the charge on metal surface atoms from -1 to +1 per atom, calculating binding energies for atomic adsorbates such as H, O, N, and C, as well as the molecular adsorbate CO on ideal single crystal 3d, 4d, and 5d transition metal surfaces, namely Cu(111), Ru(0001), and Pt(111). The applicability of each method was explored by examining the range of systems that can be calculated, computational demands, accuracy of results, and potential pitfalls. Cluster calculations, periodic methods, and implicit solvation models were compared, revealing that charged periodic calculations with homogeneous background counter charge and large vacuum region provided the most practical and computationally efficient results. The study also highlights the role of electric fields versus charge, depicting the extent of polarization of adsorbates from charge density difference plots.

Overall, the choice of method remains a tradeoff between accuracy and computational expense. The findings offer general conclusions about catalytic condensers and contribute to the understanding of electronic control in catalytic surfaces, paving the way for future advancements in programmable catalyst design.

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