

# MSE SEMINAR

Materials Science and Engineering  
Michigan Technological University

Tuesday, April 2, 2013

11:00 am – 12:00 pm

Room 610, M&M Building

## Graduate Student Presentations

### In-situ Lithiation/Delithiation Studies on Transitional Metal Oxides (TMOs) Using an Aberration-corrected Scanning Transmission Electron Microscope

**YiFei Yuan**

Graduate Student

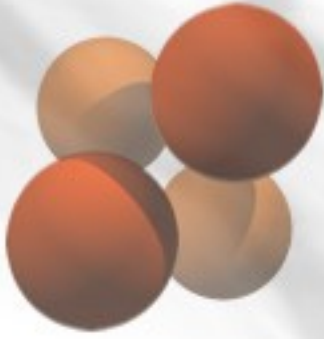
Materials Science and Engineering Dept.

Michigan Technological University

#### Abstract

Transitional metal oxides (TMOs) were recently found to offer much higher charge capacity than traditional graphite anode in lithium ion battery (LIB) mainly via a so called conversion reaction mechanism. Most TMOs, however, suffer from large irreversible capacity loss and eventually poor cycle performance, preventing its commercialization. The formation of irreversible  $\text{Li}_2\text{O}$  phase in the redox reaction is believed to lead to the poor capacity retention in TMOs. The proposed research will investigate the formation of  $\text{Li}_2\text{O}$  and its stability during half-cell lithiation/delithiation cycles in cathode TMOs ( $\text{FeO}$ ,  $\text{Fe}_2\text{O}_3$  and  $\text{Fe}_3\text{O}_4$ ) using an aberration-corrected scanning transmission electron microscopy (AC-STEM). The in-situ AC-STEM studies will be conducted inside a JEOL ARM 200CF using an electrical probe holder. Low-Angle Annular Dark Field (LAADF) and Annular Bright Field (ABF) imaging along with Electron Energy Loss Spectroscopy (EELS) will be applied specifically to trace the distribution and behavior of Li and O atoms. The results are expected to provide direct evidence of the compositional and structural change of TMOs and  $\text{Li}_2\text{O}$  during charging and discharging cycles.

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# Evaluating the Strengthening Effects of Increasing Supersaturation in Al-Sc-Zr Alloys

**Kyle Deane**  
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Materials Science and Engineering Dept.  
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## Abstract

Al-Sc-Zr alloys are known to form cored  $L_{12}$  precipitate structures upon heat treatment, with  $Al_3Sc$  nucleating and coarsening a precipitate until slower-diffusing Zr can create an  $Al_3Zr$  shell around it, limiting the coarsening and mitigating over-aging. Increasing the number density of precipitates at the optimal size through increased supersaturation will increase the strength of the material to an extent, but it will also decrease the distance between precipitates and the time it takes for Zr to slow the coarsening of  $Al_3Sc$  with a shell structure. It is therefore hypothesized that increasing supersaturation of Sc and Zr in a 1:1 ratio and performing isochronal heat treatments as proposed by Keith Knipling (2006) will reveal a peak maximum hardness after which the maximum hardness possible will decrease. Using a combination of melt spinning, powder processing, and additive friction stir processing, composition gradients will be created for efficient microhardness and WDS analysis.



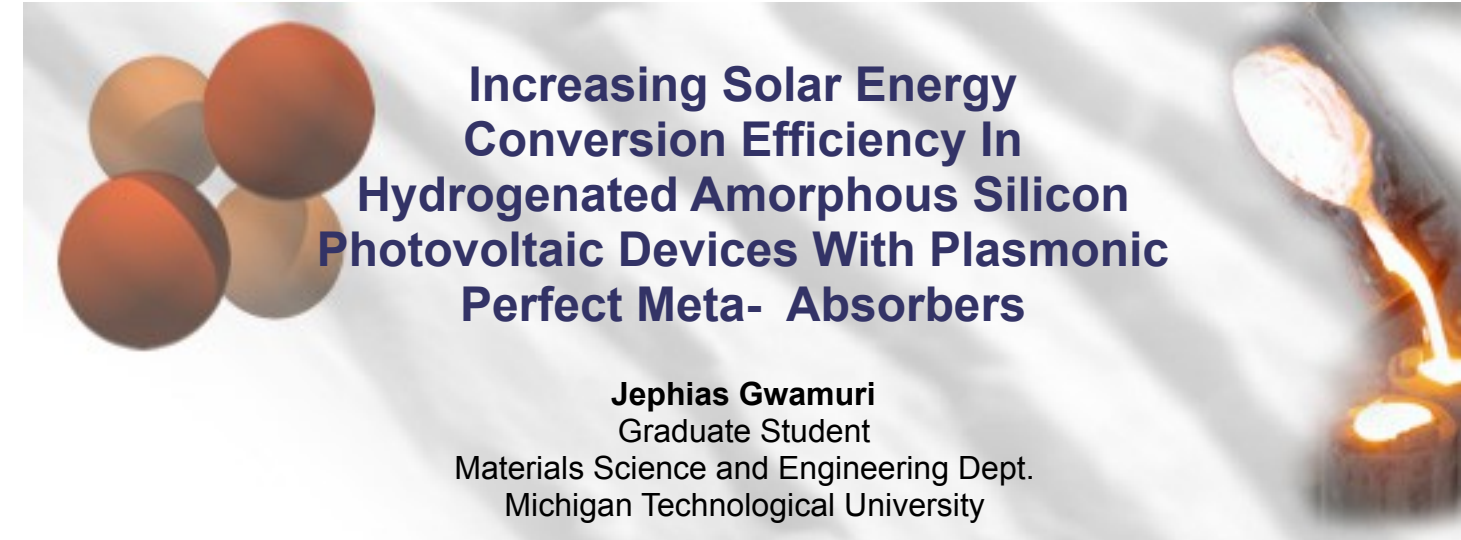
# In-Situ Mechanistic Analyses of Electrode Materials for Sodium Ion Batteries

**Jacob Kolar**  
Graduate Student  
Materials Science and Engineering Dept.  
Michigan Technological University



## Abstract

As nanotechnology and system components have improved, sodium ion energy storage systems could fill a necessary niche for large scale storage applications. Thus, it is imperative to develop more efficient materials and to further understand the systems that have been recently evaluated. With recent advances in characterization methods, the proposed research is aimed at examining the mechanistic changes that occur during sodiation/desodiation of battery electrodes, via electrochemical studies and in-situ TEM characterization. Anodic and cathodic species will be examined in an effort to further understand the principles of insertion mechanisms. Correspondingly, electrode variations will be performed and characterized with the goal of improving system performance. The proposed variables to alter are geometrical constraints, chemical compositions, and crystallographic conditions.



# Increasing Solar Energy Conversion Efficiency In Hydrogenated Amorphous Silicon Photovoltaic Devices With Plasmonic Perfect Meta- Absorbers

**Jephias Gwamuri**

Graduate Student

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## Abstract

Recent advances in optics, particularly in plasmonics and nanophotonics provide a new method to improve the optical enhancement in hydrogenated amorphous silicon (a-Si:H) photovoltaic (PV) devices and further reduce the negative effects of the Staebler – Wronski Effects (SWE). The use of plasmonic nanostructures on PV devices has been shown to enhance their efficiency . Theoretical work has indicated that absorption enhancement of up to 100% is possible for thin film PV devices using both nanostructures and metamaterials. This research project follows up on this preliminary work in trying to establish practical efficiency values in commercial grade thin film cells using resonant plasmonic nanostructures. A wide-angle polarization - independent broadband “perfect absorber” capable of achieving absorption throughout the entire AM1.5 spectrum while reducing semiconductor absorber layer thicknesses was proposed. The proposed cell design uses silver (Ag) nanostructures to create a “black” perfect absorber that can be integrated into the manufacture of commercial grade a-Si:H PV devices.

Samples of a-Si:H n-i-p test PV structures of varying thicknesses based on cells in commercial production were designed and fabricated. The n-i-p layers were optically characterized using the Variable Angle Spectroscopic Ellipsometer (VASE) from J.A. Woollam. The optical properties:  $n$  ,  $k$  ,  $\epsilon_1$  and  $\epsilon_2$  values were obtained as a function of wavelength over the entire solar spectral range for use as inputs in finite element and finite integration based optical models. Results from the optical characterization of the test cell were validated and found to be within the range of those reported by other groups. The optical parameters, were used to model an optimized plasmonic-based cell structure using COMSOL . The optimized cell consists of 200 nm Ag back contact, a 100 nm aluminum doped zinc oxide (AZO) layer, 300 nm a-Si:H layer, 30 nm thick (120 nm wide) Ag grating nanostructures and 60 nm thick antireflecting coating (ARC). Synthesis of the optimized Ag grating nanostructures is in its initial phase using resources from the Michigan Tech Microfabrication facility and lithographic resources available through the National Nanotechnology Infrastructure Network (NNIN) at UT-Austin/ UIC/UM/UW) if it became necessary. The finished cell will be tested for both optical and photocurrent enhancement using both spectral response and a class AAA solar simulator. Device performance results will be fed back into the models to help refine and optimize the plasmonic enhanced a-Si:H PV devices. Achieving record device performance and overcoming design and fabrication challenges will help thin film a-Si:H solar cell compete with other mature technologies such as monocrystalline and tandem solar cells which have recorded efficiencies greater than 30% at one sun.

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