Imaging Perovskite Materials At The Atomic Scale Using Synchrotron X-ray Scanning Tunneling Microscopy

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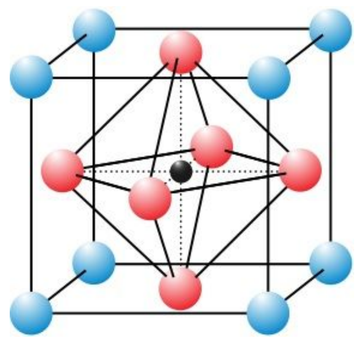
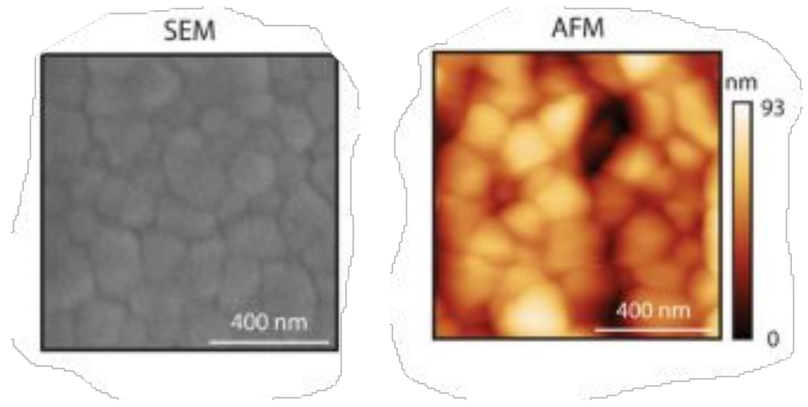
MOTIVATION

- As population increases, and with the demand for solar energy greater than ever for developed countries, perovskite solar cells have the potential to be a less expensive and more efficient alternative to silicon solar cells.
- Perovskites are not very stable and only last a year at most, whereas silicon solar cells can last for 25 years or more.
- The purpose of this experiment is to try to understand the mechanisms of the degradation of perovskite solar cells under conditions that simulate their operation in the field. Using Synchrotron X-ray Scanning Tunneling Microscopy we monitored the electromagnetic configuration of the perovskite to look for potential degradation



Perovskite Crystal Structure[1]



MAJOR ACCOMPLISHMENTS

- In this experiment, we studied a novel perovskite formulation $(Cs_{0.05}(FA_{0.83}MA_{0.17})_{0.95}Pb(I_{0.83}Br_{0.17})_3$ using the synchrotron x-ray n order to observe the effect of applied voltage and incident visible light (λ= 550 nm) on the iodine M4,5 absorption edge under conditions where voltage was applied to the sample and where light was incident on the sample.

- The x-ray examines the electromagnetic organization of the materials at the nanoscale level in order to simulate real-world use of the perovskite material. Using the spectroscopic capabilities of the beamline, and probing the M4 and M5 absorption edges in the iodine atoms of two different perovskite compositions; We were able to observe the electromagnetic configurations in order to detect potential degradation.

- In figure 1, we study how the effect of applying a voltage to the perovskite effects the makeup of the M 4,5 iodine absorption edges. In our spectra, we noticed that the shoulder at 642 eV becomes less distinct as applied voltage increases and the peak at 650 eV begins to flatten. We concluded that the structure and position of the absorption nearly remains the same when we have low voltages applied. However, there is a small shift of the rising edge feature to higher energies.

- In figure 2, we are observing the effect of applying a monochromatic light to the perovskite while observing the M 4,5 iodine edge. In our spectra, we notice that the shoulder appears at about 665 eV and the peak at 652 eV becomes more pronounced.

Figure 1 - Iodine M 4,5 Absorption Spectra - Comparing Bias Voltage

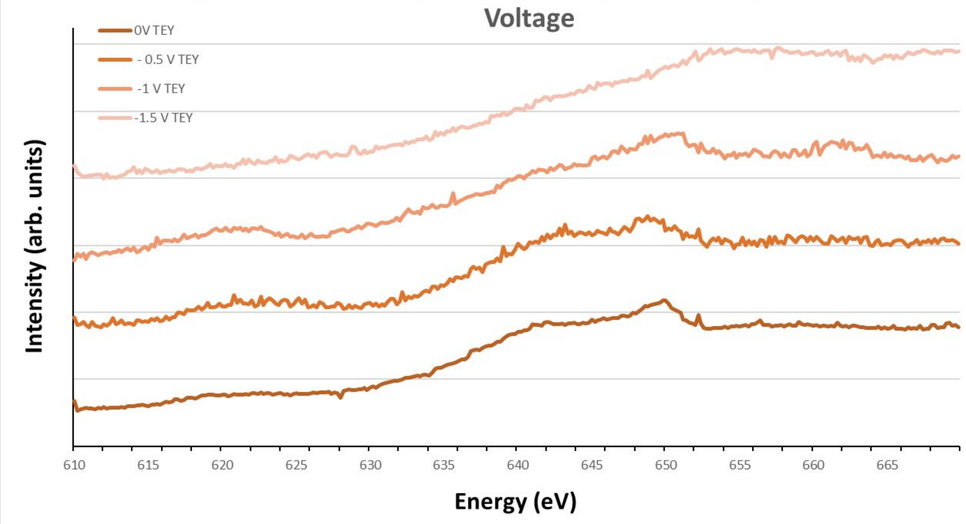
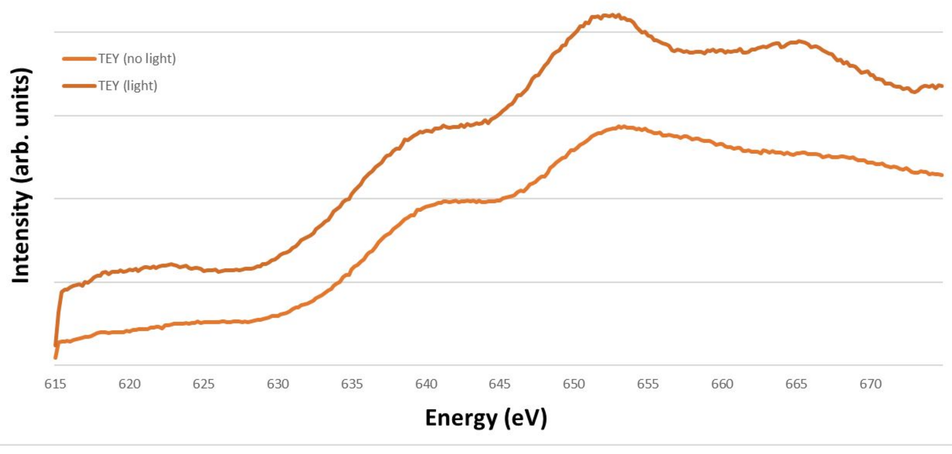


Figure 2 - Iodine M 4,5 Absorption Spectra - Comparing Illumination



IMPACT

- We observe that the impact of light is much stronger compared to voltage. One hypothesis is that charged defects can accumulate at the interface, changing the local polarity under an applied voltage. There may also be a change in the octahedral structure and bond length.

- These results can be contrasted with our previous results for a more typical perovskite formulation ($MA_xFA_yPbI_3$ ($methylammonium_x$ $formamidinium_y$), which showed that both the energy and peak height of the M4 and M5 absorption edge of iodine shifted more noticeably under an applied voltage.

FUTURE DIRECTIONS

- Replicate this experiment using more typical perovskite formulations to determine if light has similar effects on these samples.
- Run experiments on perovskites that have been used in the field to see what effect being subjected to varied real world conditions have on the chemical bonding and octahedral structure of the material. This could be combined with transmission electron microscopy measurements to further illuminate any crystallographic changes of the perovskite as it is used in a photovoltaic cell.
- Expand the parameters of the current experiment through the use of different wavelengths of visible light and increased voltage to determine the effects of higher photon energy and charge on the degradation process in regards to the efficiency of the perovskite solar cell.
- Formulate and experiment with novel perovskite combinations to test the efficiency and resilience of other elements.

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