Optical Characterization of Thin Film $BaZrS_x$

Athalia Meron, athmeron@gmail.com
Harvard-Westlake School, Class of 2021
USC Viterbi Department of Chemical Engineering and Materials Science, SHINE 2020

Introduction

Perovskites are a class of material with the general form ABX_3, giving them a unique crystal structure. Their specific structural composition gives them highly tunable chemical and physical properties, making perovskites highly versatile. Due to their unique properties, they are promising for a variety of applications, including optoelectronics.

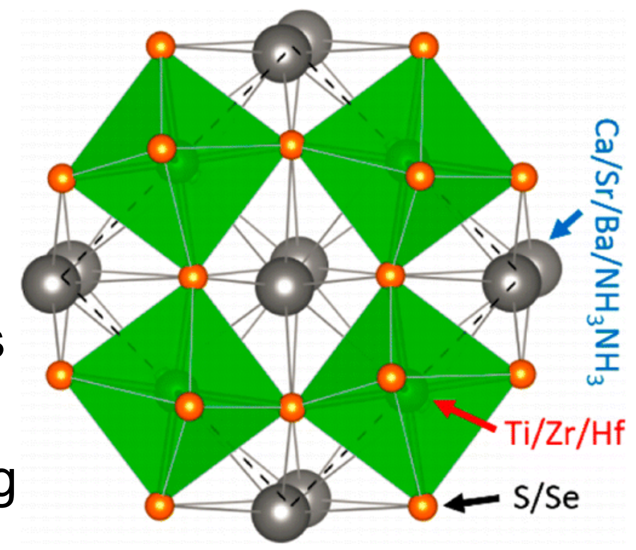

Fig. 1: Perovskite Crystal Structure PC: Sun et al., 2015, "Chalcogenide Perovskites for Photovoltaics", published in Nano Letters (pubs.acs.org/NanoLetters)

Objective & Impact of Professor's Research

Professor Ravichandran's research focuses on the synthesis and characterization of complex materials such as transition metal perovskite oxides and chalcogenides (containing an S, Se, or Te atom). Specifically, my PhD mentor's work centers around the characterization of these materials, as well as optimizing processing conditions to make devices, such as solar cells from these materials.

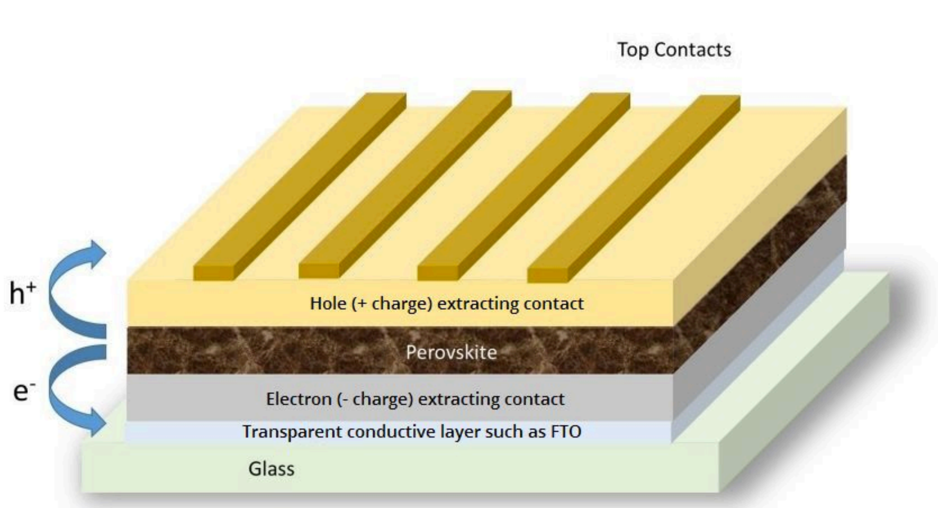

Fig. 2: Cross section of a perovskite solar cell PC: Clean Energy institute (https://www.cei.washington.edu/education/science-ofsolar/perovskite-solar-cell/)

Optical Characterization

Professor Ravichandran's lab had previously synthesized bulk crystals of $BaZrS_x$ (BZS), a novel perovskite chalcogenide material. More recently, they have synthesized thin films of BZS and are in the process of characterizing the material. Since one of the goals of Dr. Ravichandran's lab is to produce optoelectronics from these new materials, it is important to know how they interact with light. Optical characterization employs a variety of spectroscopic methods to determine the materials' optical and electrical properties, which then inform processing conditions for these devices. I analyzed different data spectra to determine some of the BZS material properties.

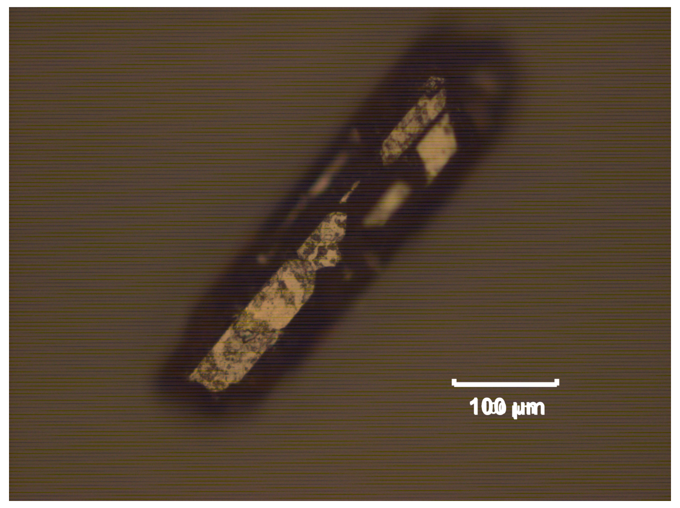

Fig 3. A Ba_2ZrS_4 Crystal PC: Huandong Chen

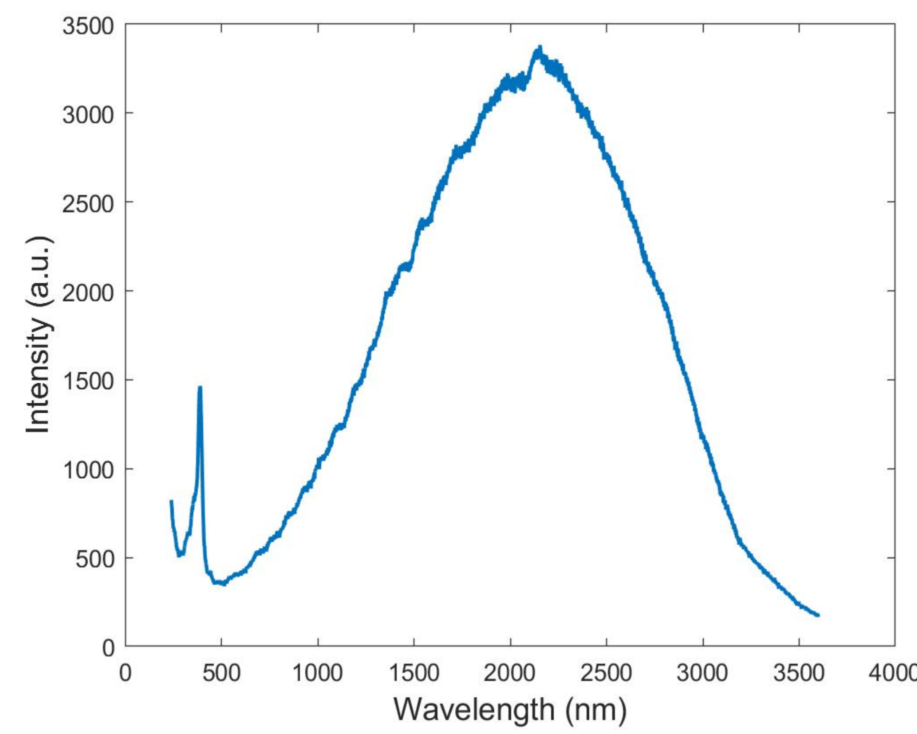

Fig 4. PL Emission Spectrum of bulk crystal 2:1:4 BZS PC: Athalia Meron

I. Photoluminescence Spectroscopy (PL)

Light of various different wavelengths is shined onto a sample and the excitation at each wavelength is measured. The excitation spectra give us important information about the optical bandgap of the material, as well as information about crystallinity and film quality.

II. UV-Vis Spectroscopy

White light is shined from a source onto the thin film sample, and we are able to measure the transmittance and reflectance of the film by detecting how much light was reflected off of the surface or absorbed. Using this information, we can extract information such as the material's absorption coefficient and bandgap energy, as well as the film thickness. These data give us information about the film's quality and optical properties, which inform processing conditions for device fabrication from these materials. Here, the absorption band edge is around 500 nm, indicating a bandgap of 2.5 eV. Given that the bandgap is fairly large, the film may be amorphous or have imperfect stoichiometry, indicating that the synthesis conditions should be refined.

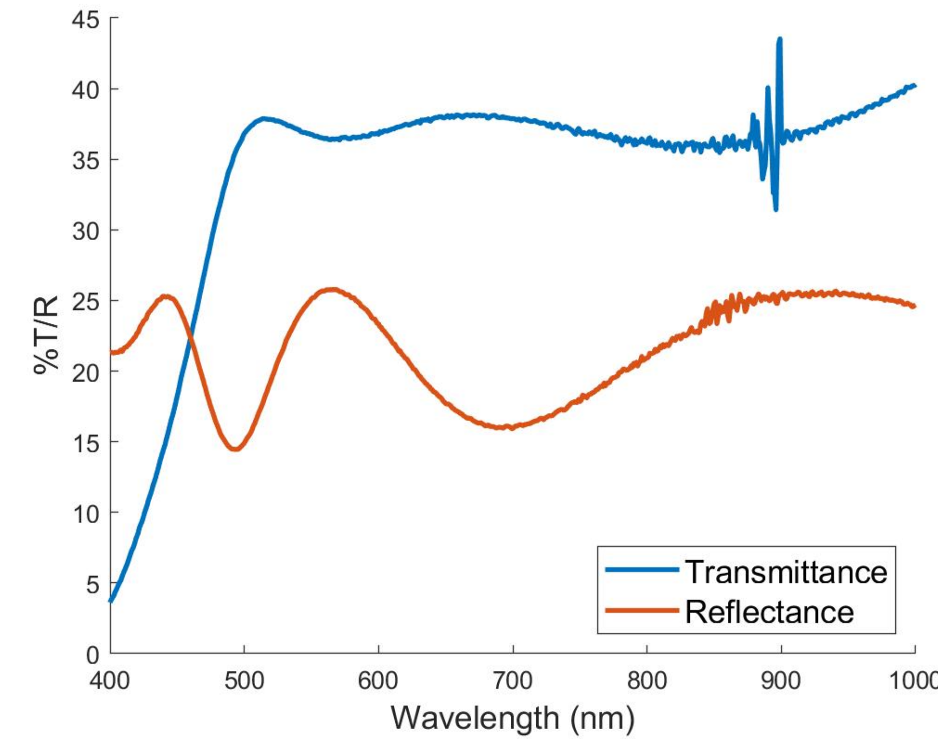

Fig 5. Reflectance and Transmittance Spectra from Thin Film BZS. PC: Athalia Meron

How This Relates to My STEM Coursework

Working in Professor Ravichandran's lab has exposed me to more advanced data analysis techniques that I will be able to apply in future STEM courses. I've been exposed to a variety of different materials characterization methods. While each method is unique, they all relate to spectral analysis, which is an extremely flexible skill that I am excited to take forward with me into further STEM courses. Additionally, I've learned to visualize data using MATLAB,.

Next Steps

- Regrow films under different conditions to improve stoichiometry
- Continue characterizing using different methods, including different chemical, structural, and electrical characterization methods

Acknowledgements

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