Characterization and Modeling of $BaZrS_3$ for Photovoltaic

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Introduction

A perovskite structure is a specific structure that has the chemical composition of ABX_3. It is characterized by the octahedral structure formed by BX_3 in the center with A atoms in the corners. Ruddlesden-Popper (RP) phase is an intercalating structure of ABX_3 perovskite which has the chemical composition $A_{n+1}B_nX_{3n+1}$.

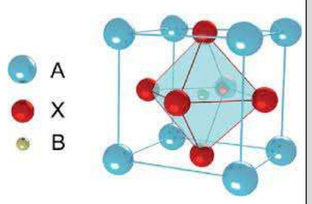

Figure 1. Perovskite crystal structure

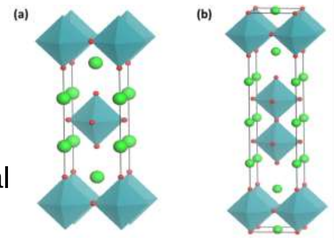

Figure 2. RP phase structure

Objective & Impact of Professor's Research

The objective of professor Ravichandran's research is to synthesize and identify novel semiconductors for electrical and optical applications. The material that is currently being looked into is the perovskite $BaZrS_3$ and its RP phase. The potential impact of this research is that $BaZrS_3$ can be a good candidate for fabricating high efficient photovoltaic devices. This would lead to a better harvesting of solar energy.

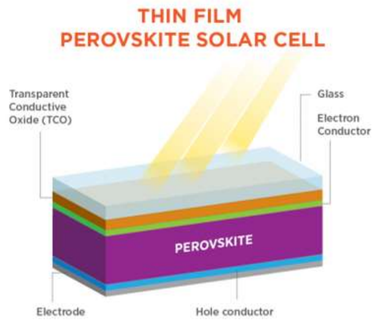

Figure 3. Model of a perovskite solar cell

X-Ray Diffraction (XRD)

XRD is a technique that allows for the characterization of material structures. It also gives information about the crystallinity such as its texture, orientation, and defects. Powder XRD was used in our research to compare $BaZrS_3$ and its RP phase that was synthesized by its stoichiometry with the corresponding standard structures.

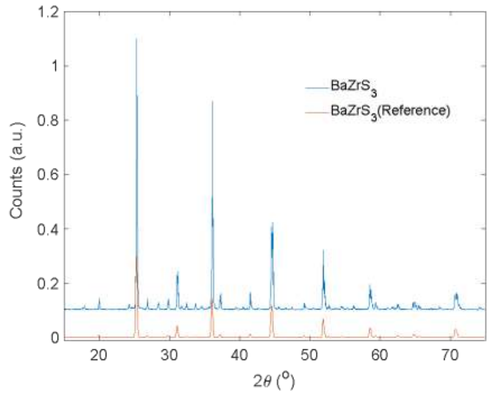

Figure 4. X-ray diffraction of $BaZrS_3$ and reference data.

The synthesized $BaZrS_3$ matches well with the $BaZrS_3$ standard structure.

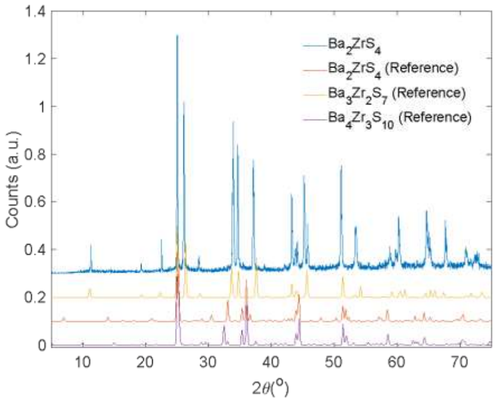

Figure 5. X-ray diffraction of Ba_2ZrS_4 and reference data.

I was able to identify that the crystal structure of our synthesized RP phase was Ba_2ZrS_4 by comparing powder XRD with different RP phases of $BaZrS_3$.

Heat Conduction

Heat conduction can be modeled using the equation $\rho c\, \partial T/\partial t = \nabla\cdot(k\nabla T) + \alpha Q$. We are trying to use this equation to simulate real circumstances in a photoelectric measurement. It can be visualized by using a visible laser to illuminate a crystal, generating electrons and holes. This also causes the illuminated area to heat up. By studying the heat dissipation in this crystal, it is possible to learn how efficiently a material is able to conduct and transfer heat. The aim of this procedure is to calculate the heat dissipation of materials that are being researched.

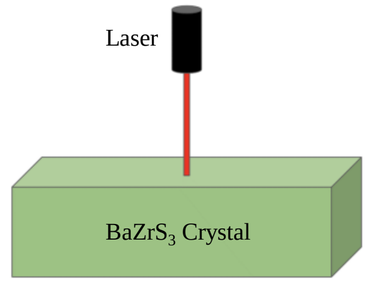

Figure 5. Basic laser heating model.

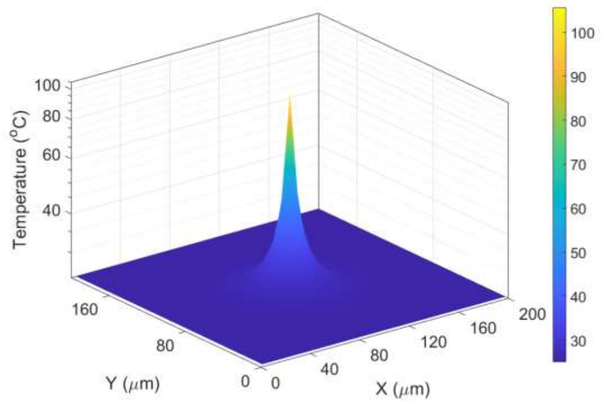

Figure 6. Temperature profile of top surface of $BaZrS_3$ crystal

The laser hits the top surface of the crystal, creating a local heating area. The temperature drops sharply as we diverge from the heating area.

Next Steps

$BaZrS_3$ and its RP phase is predicted to work and we are going to demonstrate such photovoltaic device. We will do more research on the electrical conductivity of the material and the photoelectric effect. The growth of BaZrS3 thin film will give us access to functional photovoltaic devices.

Skills learned

Many of the skills I learned throughout my time at SHINE pertains to coding. For example, Matlab and Python were some programs that I learned to use. I also learned how to read and search for scholarly articles.

Conclusions

By using techniques like XRD, we are able to characterize the nature of $BaZrS_3$ and its RP phase. Heat dissipation model allowed us to identify the temperature change during laser illumination. These results help us understand the photovoltaic phenomenon of this material and provide vital information for photovoltaic applications.

Acknowledgements

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