Visualization of Cathode Material

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Introduction

With the current intercalation materials, repeated use of active ions in the material cause strains to the crystallographic texture, found in most rechargeable batteries. By analyzing the crystallographic structure and finding the flaws, the material behavior can be enhanced. This would fix the structural integrity in order to make the batteries lifespan stronger.

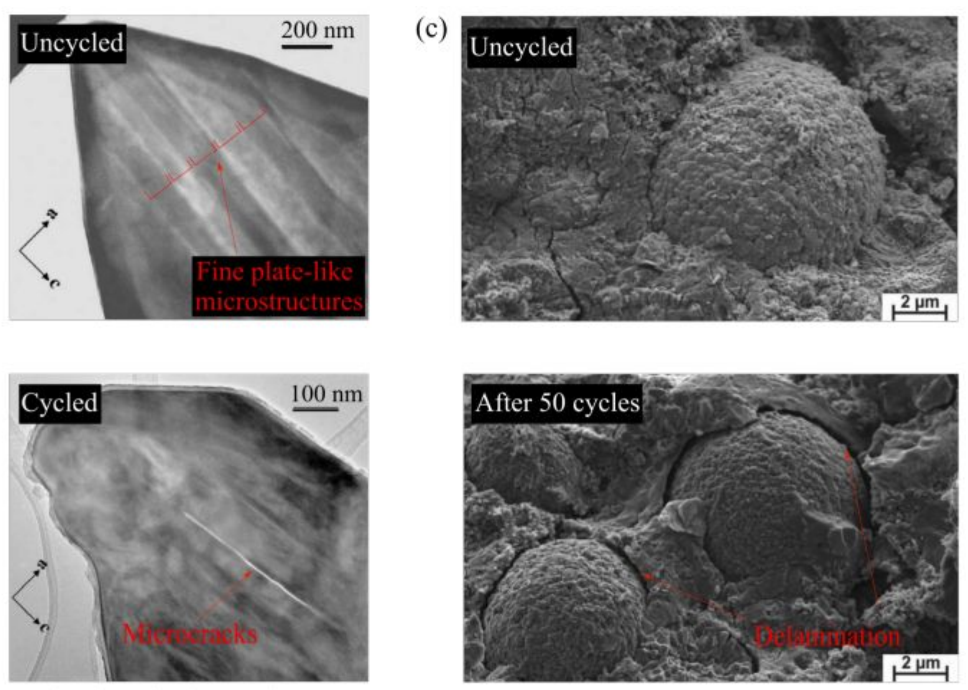

Figure 1. Intercalation material before and after being cycled
Photo Credit: Professor Renuka Balakrishna

Objectives & Impact of Professor's Research

Professor Renuka Balakrishna's research involves intercalation, which occurs after active ions are inserted and a cycle is created. This has allowed for better rechargeable batteries that undergo this cycle. Although the intercalation materials provide a better solution, they are avoided because when they undergo multiple structural changes, they begin to degrade. By looking at how these materials behave it may be possible to find a solution, to prevent rechargeable batteries from deteriorating.

Lattice Structures

Simple Cubic is a crystalline structure with lattice points at each corner.

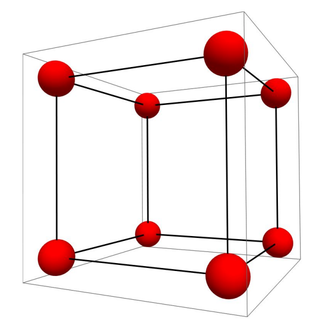

Figure 2. Model of Simple Cubic

Face Centered Cubic is a crystalline structure with lattice points at each corner with additional ones of each center of the faces of the cube.

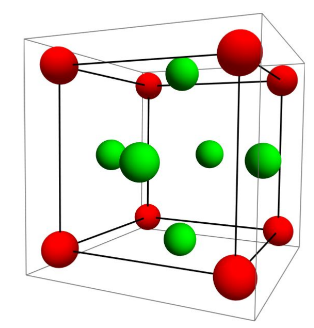

Figure 3. Model of Face Centered Cubic

Body Centered Cubic is a crystalline structure with lattice points at each corner as well as one at the middle of the cube.

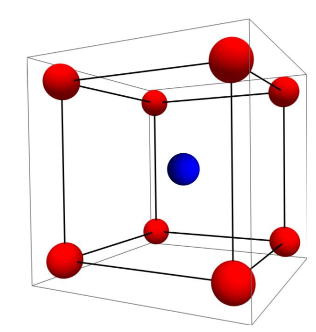

Figure 4. Model of Body Centered Cubic

These structures are used in to increase surface area and distribute material effectively.

Intercalation Material

An intercalation material located in the cathode is LiV_2O_5 . Using Mathematica I was able to visualize after getting the coordinates of each atom. This was done by multiplying the original coordinates by the relative coordinates. The X, Y and Z coordinates all had to undergo this process. Later in Mathematica they were graphed in order to produce the material shown in Figure 5.

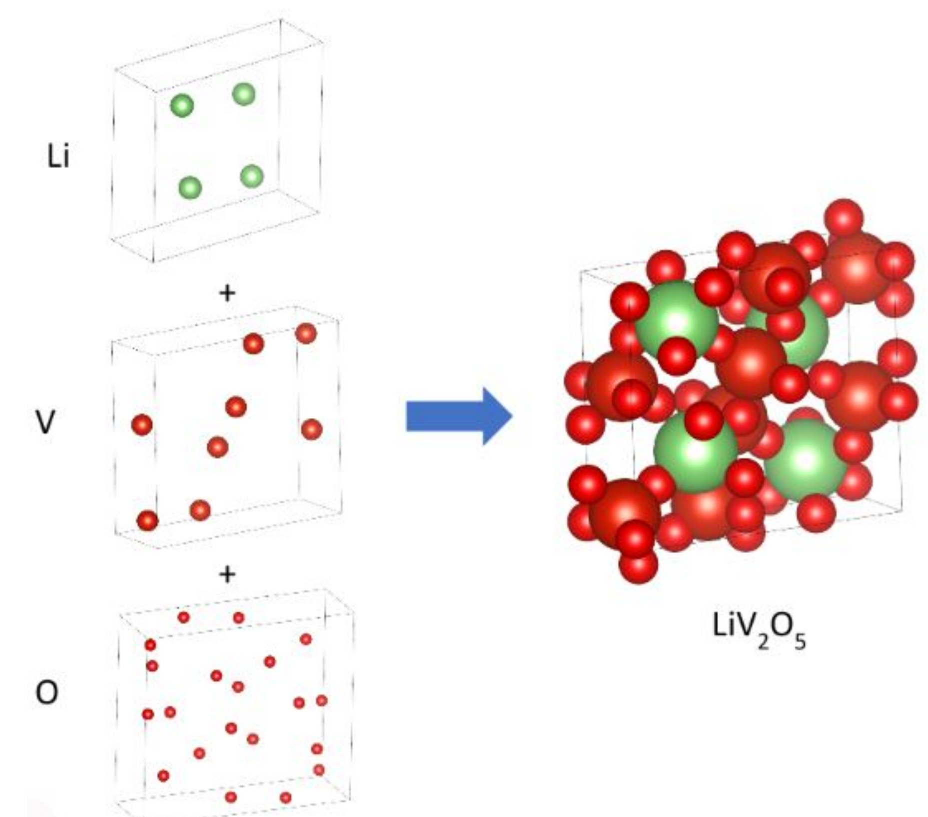

Figure 5. Visual representation of LiV_2O_5
Photo Credit: Delin Zhang

How This Relates to Your STEM Coursework

The SHINE experience impacted my STEM understanding in the best way possible. I learned new things, such as the base to use Mathematica, which is used in college. I also have an understanding of how research works at the college level. My SHINE experience definitely makes me more interested to learn more and my newfound curiosity in certain topics will continue in my education.

Figure 6. Mathematica logo
Photo Credit: wikipedia.com

Next Steps for You and Advice for Future SHINE Students

The next steps on my STEM journey would be to finish my senior year, and continue at a college. I would like to continue learning more about engineering and the different aspects. Being a part of SHINE, definitely allowed me to learn about the different fields of engineering and has encouraged me to try and incorporate it in my future studies.

Skills Learned

- ❖ I was able to learn how to use Mathematica in different ways, one of which being for this research project.
- ❖ In the beginning it was challenging but after completing smaller projects I gained more experience and knowledge.
- ❖ As a result I gained more confidence in using Mathematica to complete the tasks given.

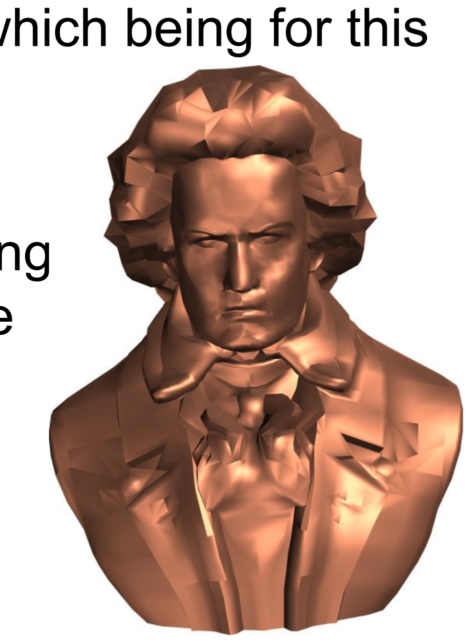

Figure 7. One of the many things Mathematica can do

Acknowledgement

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References

Zhang, Delin, and Ananya Renuka Balakrishna. "Designing shape-memory-like microstructures in intercalation materials." arXiv preprint arXiv:2206.14948 (2022).