Sythesis of Transtion Metal Halides: Discovering Ferroelectric Materials

Bianca Brown.[1] Tyrel McQueen[2], Nicholes Ng[3]

Clark Atlanta University

ABSTRACT

Ferroelectricity which have switchable dipole moments are capable of improving internal potential and output power of energy. They are used in advanced technologys as well as electronical devices such as phones, and computers. Our goal is to create a new type of flexible ferroelectric substrate that can be used to inhance the power efficacy of technology and new types of devices. In this study, I am focusing on 2D inorganic ferroelectrics that can be used as a templet for the self-assemble of organic substrates. Creating new types of ferroelectric materials that are using Nb_3Cl_7X,(X=S,Se,Te), materials which will be prepared and tested for ferroelectric behaviors.

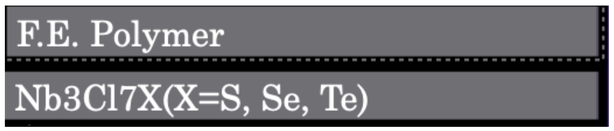
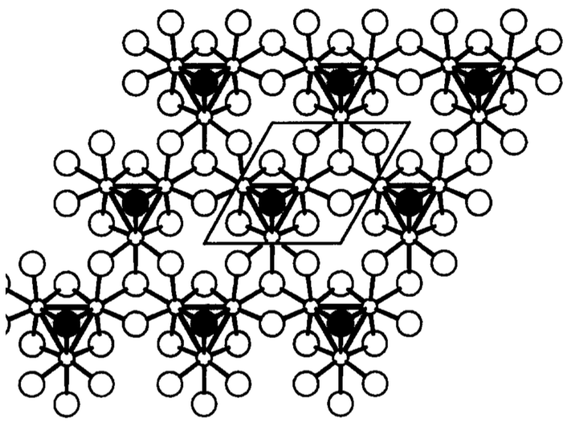


Figure 1. Material to be formed



. 2. (001) projection of a single layer of Nb_3TeCl_7: ○, Nb; ●, Te; Cl.

Figure 2. Polar Niobium

INTRODUCTION

The goal of my project here at PARADIM is to create a ferroelectric material that can serve as the template for the self-assembly of organic ferroelectric polymers which may possess superior electrical properties, with potential uses in advanced devices. I will be focusing on 2D inorganic ferroelectrics that can be used as a template for the self assembly of organic materials.
This relates to my study back at my home school in the sense that while I know how to synthesize 2D inorganic templetess and the targeted organic polymers, we are hoping to expand on that synthesis and create a flexible material that can have ferroelectric properties.

METHODOLOGY

To be able to crate and study Nb_3Cl_7X,(X=S,Se,Te) a single crystal structure must be created by Chemical Vapor transport, CVT. CVT is the process of taking a transport agent and a condensed solid phase and creating a crystal on the opposite end of the temperature gradient.[1] To produce larger crystals using a multizone furnace in which you can control the temperature gradunt as well as increasing the transport rate. Leaving the reaction for roughly three to four day and then running XRD and SEM to check what was created from the CVT.Temperaure gradient of 820C, 785C , with the third zone at 795C.

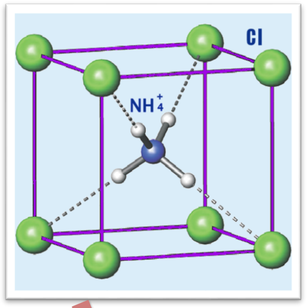


Figure 3. Ammonium chloride

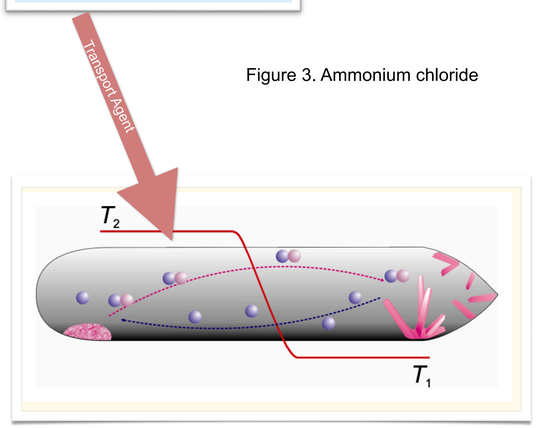


Figure 4. Chemical Vapor Transport growth

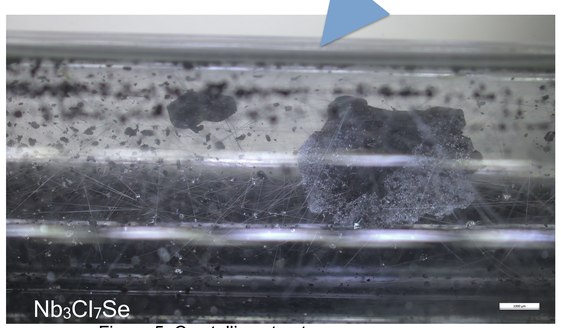


Figure 5. Crystalline structure

RESULTS

They where left for three days and then ramped back down to room temperature and was then ready for XRD and Scanning Electron Microscope,SEM test. Energy-dispersive detector,EDS/EDX gave the accurate ratio of Nb3Cl7Te but Nb3Cl7X(X=S, Se) have impurites.

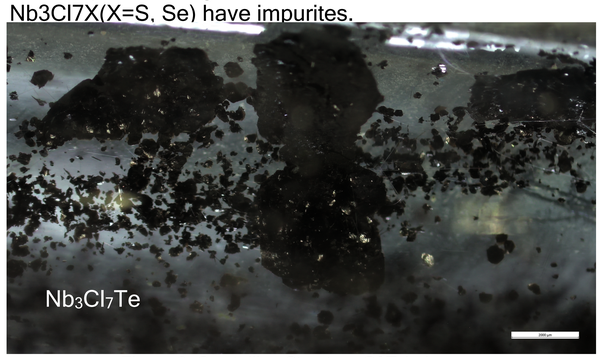


Figure 6. Crystalline Structure Of Telerium

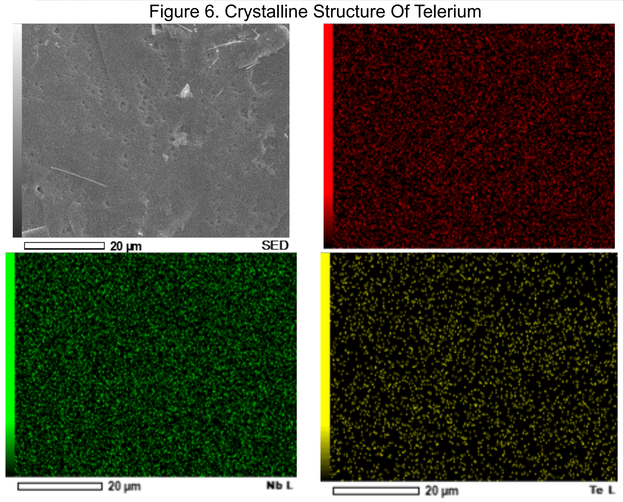


Figure 7 .A homogenous structure was formed by Nb3Cl7Te.

Interpritations

- My initial results are contaminated by air, causing oxygen,Nb3O to infiltrate my reaction chamber.
- To optimize the reaction I'm purifying to remove oxygen.
- Once I have successfully made larger samples of my target materials, I will then attach contact leads and make an equivalent capacitor and then attach to a voltmeter to measure their electrical properties.

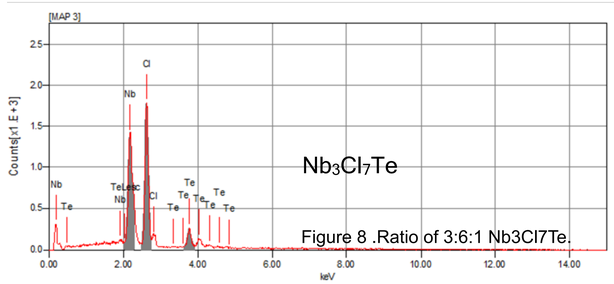


Figure 8 .Ratio of 3:6:1 Nb3Cl7Te.

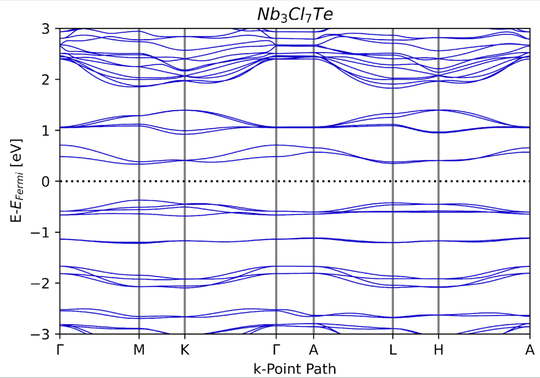
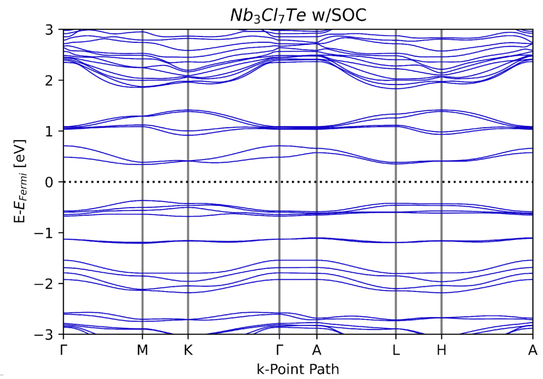
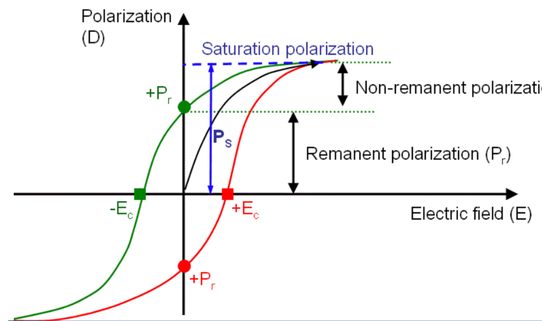


Figure 9 .10: Band Structure with bad gap of no change. 0.7107eV to 0.7105eV



Next Steps

Using the Physical Property Measurments, PPMS, to identify if my materials contain their own electrical current. Watching for the hysteresis loop. Updating and purifying the ratio of Te:Cl.



ACKNOWLEDGEMENTS

Thank you Prof. McQueen, Nicholes Ng, Thomas Whorisky. This material is based upon work supported by the National Science Foundation (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-2039380, and the REU program NSF DMR-2150446.
The Vivian Thompson Scholorships.
Reu Counterparts
McQueen Lab

1. *Chemical vapor transport*. Mpg.de. https://www.cpfs.mpg.de/2651362/chemical-vapor-transport. (accessed 2022-07-18).

2.Globalsino.com. https://www.globalsino.com/EM/page3544.html (accessed 2022-07-18).

3.Miller, G. J. Solid State Chemistry of Nb3Cl8: Nb3TeCl7, Mixed Crystal Formation, and Intercalation. J. Alloys Compd. 1995, 217 (1), 5-12. https://doi.org/10.1016/0925-8388(94)01298-v.