

# Studying Non-Trivial Atomic-Scale Heterostructures

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## 1 Introduction

The goal of this project is to create thin film heterostructures. This will be done by using pulse laser deposition (PLD). A thin film can range in different thicknesses. This range can be from nanometers to several micrometers. An example of a thin film that is more commonly known includes soap bubbles and a type of anti-reflection coating on eyeglasses. [2]

The properties of thin films can change based on the amount of oxygen in the structure. Some thin film heterostructures have semiconductive behaviors. [4] Semiconductors are very common today because they can be found in many electronic devices. This includes phones, laptops, tablets, calculators, game systems, Televisions, radios, smart devices, and more. It is important for these semiconductors to be thin in size. The reasoning behind this is that our technology today continues to get thinner and thinner in size. If smart devices and technology continue to get thinner, the materials that make up these devices would also need to get smaller and thinner. This is why thin film heterostructures are so important. The crystal structure of Strontium Cobaltite (SCO) is important because of its semiconductive behaviors. There is a lot of interest in the field of thin film heterostructures because of its potential of out performing conventional semiconductors. [3] The thin film of Strontium Carbonate is also an antiferromagnetic insulator. [6] There is currently a major interest in antiferromagnetic insulators due to its abilities of storing information onto these thin films. This new discovery helps with our current technology advancements. As devices continue to get smaller and smaller, these thin films can help keep up with this trend since they can store information and are very thin and small. [5]

This experiment will focus on creating thin film  $\text{SrCoO}_{2.5}$  by using pulse laser deposition. Using the powdered substances Strontium Carbonate,  $\text{SrCO}_3$ , and Cobalt (II, III) Oxide,  $\text{Co}_3\text{O}_4$ , this will be used to create Strontium Cobaltite,  $\text{SrCoO}_{2.5}$ . The crystal systems for the different powders are orthorhombic for the  $\text{SrCO}_3$  and tetragonal for the  $\text{Co}_3\text{O}_4$ . The crystal system for the product,  $\text{SrCoO}_{2.5}$ , is orthorhombic. Using the Strontium Carbonate and Cobalt (II, III) Oxide in the correct ratios, conditions, and equipment, Strontium Cobaltite will

form. The correct ratios can be determined by balancing a chemical equation and the mixture of the Strontium Carbonate and Cobalt (II, III) Oxide to create the Strontium Cobaltite. The ratio of what is needed to create the Strontium Cobaltite from the Strontium Carbonate and the Cobalt (II, III) Oxide is 3:1 which is three parts Strontium Carbonate and one part Cobalt (II, III) Oxide. The  $\text{SrCoO}_{2.5}$  becomes a polycrystalline after the use of PLD.

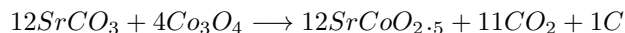
A method being used in this experiment is X-ray Diffraction, XRD. X-ray diffraction can find the crystallographic structure of a crystal. It can also determine any impurities in a material. This includes its crystal structure, size, and what type of crystals are present. This method can be done by using incident X-rays and measuring the waves present and the different scattering angles of the X-rays that leave the material. The XRD will also be used to check the properties and changes of the powdered sample when calcined and sintered. It will then be compared with theoretical XRD graphs using a program called VESTA.

After the Strontium Cobaltite crystal is formed using PLD, another technique will be used called Atomic Force Microscopy, AFM. This is used to measure the surface topology of a substance or material and view how the surface looks, or its topology. For example, the AFM can determine if the surface of a material is hilly, smooth, etc. This allows imaging of many different types of surfaces. It can do this by using three methods. The methods are contact mode, non-contact mode, and tapping mode. Contact mode is done when the tip of the cantilever makes very close contact with the surface. This method is used when measuring surface force. Non-contact mode is done by keeping the probe several nanometers away from the surface in a spot with interaction forces. The last method and the method that will be done for this project is tapping mode. This method is done by vibrating near the fundamental resonance frequency and the tip of the probe moves up and down. The tip only sometimes comes into close contact with the surface.

There is a lot of interest and research in the field of semiconductors and thin film heterostructures. The formations, physical properties, and structural properties of these crystals and their potential applications as solid-state fuel cells. [4]

## 2 Procedure

The method of creating the strontium cobaltite starts with the powders Strontium Carbonate ( $\text{SrCO}_3$ ) and Cobalt (II,III) Oxide ( $\text{Co}_3\text{O}_4$ ). The balanced equation for this reaction is as follows:



Now that the equation is balanced, stoichiometry can be used to find out how much of each powdered reactant is needed to create the target amount of grams of the product,  $\text{SrCoO}_{2.5}$ . For this experiment, two grams of the product

is being created. This means that 1.5827 grams of  $\text{SrCO}_3$  and 0.8605 grams of  $\text{Co}_3\text{O}_4$  will be used to create 2 grams of  $\text{SrCoO}_{2.5}$ .

Next, X-ray diffraction is used to confirm that the powdered reactants are free of impurities. The XRD will be used twice during this step. Once to test the  $\text{SrCO}_3$  and again to test the  $\text{Co}_3\text{O}_4$ . After the use of the XRD, the data and peaks from the machine need to be compared with the theoretical XRD data. If the peaks do not match, then the powder is impure. The conditions for the XRD was set with a start angle of  $10^\circ$  and an end angle of  $100^\circ$ . The step size is  $0.02^\circ$ . The speed was set for  $1.0^\circ/\text{min}$ .

Then, when the powders are proven to be pure and free of impurities, the next step is to mix and grind the powders together. This is done by putting the powders in a mortar and grinding it with a pestle. Grind the powders together until fully mixed and finely grounded. For this project, the powders were mixed together for 40 minutes.

After the powders are finely grounded, the mixture should be placed in a crucible to be placed in a furnace. The  $\text{SrCO}_3 + \text{Co}_3\text{O}_4$  should be calcined in a furnace for  $900^\circ\text{C}$  for six hours. This process helps remove possible volatile substances and it can oxidize a portion of the mass. This step is a method of purification. [1]

The pellet can be molded by putting the calcined powder into a dry pellet pressing die. This pellet die helps the powder get formed into a pellet. The powder should get grounded again for 40 minutes using the mortar and pestle and then put into the pellet die. After that, the pellet die should be put into a hydraulic press using 20,000 pounds of pressure for 60 minutes. Next the pellet should be carefully taken out of the die and then placed into a crucible.

Finally, the pellet that was placed in the crucible should then be placed in the furnace at  $1100^\circ\text{C}$  for 24 hours.

### 3 Discussion

The XRD graphs of the  $\text{SrCO}_3$  and the  $\text{Co}_3\text{O}_4$  powders were shifted a bit to the right more and more after each peak when compared to the theoretical XRD graphs.

As you can see in figure 1, it shows the theoretical XRD data for  $\text{Co}_3\text{O}_4$ . As the x-axis continued to increase, the shift also increased between the peaks. This can be seen in figure 2 with the data from the XRD and comparing it with figure 1 that has the theoretical XRD for  $\text{Co}_3\text{O}_4$ . The XRD for  $\text{Co}_3\text{O}_4$  also found a possible impurity that can be seen in figure 1. There is a peak that should not be there. This is the peak between the 111 and 220 miller indices.

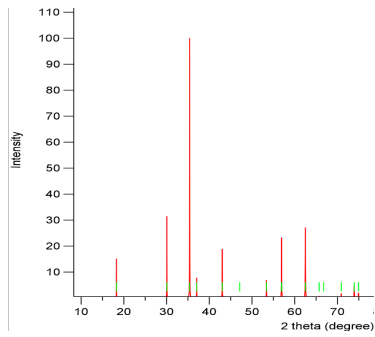


Figure 1: Theoretical XRD of Cobalt (II,III) Oxide ( $\text{Co}_3\text{O}_4$ )

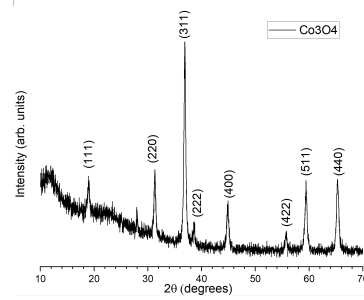


Figure 2: XRD of Cobalt (II,III) Oxide

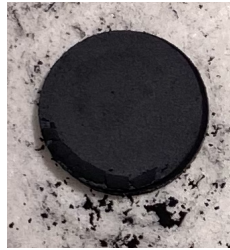


Figure 3: Pellet of  $\text{SrCO}_3 + \text{Co}_3\text{O}_4$  after in press at 20,000lbs. for 60 minutes.

When using putting the powders in the pellet die and then under the hydraulic press, the pressure was set for 36,000 lbs. This made the sample very fragile and made it not hold its shape as seen in figure 4



Figure 4: Pellet of SrCO<sub>3</sub> + Co<sub>3</sub>O<sub>4</sub> after in press at 36,000lbs. for 60 minutes.

For the second attempt, 20,000lbs. of pressure was used. This made the pellet less fragile and it still kept its shape as seen in figure 3. The pellet was sintered to help make it more dense while maintaining its properties.

The next steps are to check the structure and properties of the pellet and then to use it as a target for the PLD to create the thin film.

## References

- [1] “Calcination”. In: *Britannica Encyclopedia* (2021).
- [2] “Exploring Materials—Thin Films”. In: *NanoDays* (2010).
- [3] Weiwei Li, Kelvin H. L. Zhang Jueli Shi, and Judith L. MacManus-Driscoll. “Defects in complex oxide thin films for electronics and energy applications: challenges and opportunities”. In: *Royal Society of Chemistry* (2020).
- [4] Youwen Long. “Synthesis of cubic SrCoO<sub>3</sub> single crystal and its anisotropic magnetic and transport properties”. In: *Journal of Physics: Condensed Matter* (2011).
- [5] Universitaet Mainz. “Storing information in antiferromagnetic materials”. In: *phys.org* (2020).
- [6] Jiali Zhao et al. “Manipulating the Structural and Electronic Properties of Epitaxial SrCoO<sub>2.5</sub> Thin Films by Tuning the Epitaxial Strain”. In: *ACS Publications* (2018).