

**Title:** Preparation of SrVO<sub>3</sub>/SrTiO<sub>3</sub> (001) Epitaxial Thin Films by Pulse Laser Deposition

**Author:** Tina Tong

**Date:** August 12, 2022

## **Abstract:**

Strontium vanadate, SrVO<sub>3</sub> (SVO), is a cubic perovskite that exhibits highly conductive behavior making it a candidate as a transparent conducting oxide (TCO) [1]. Furthermore, SrVO<sub>3</sub> being a highly correlated material means that when it is doped or reduced in dimensionality, it undergoes metal-insulator transition (MIT), this property makes SrVO<sub>3</sub> of great interest to research [2,3,4]. This experiment aims at synthesizing a SrVO<sub>3</sub>/ SrTiO<sub>3</sub> epitaxial thin film by Pulse Laser Deposition (PLD) using Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> as the target and SrTiO<sub>3</sub> (001) as the substrate. While the deposition was successful, the quality of the thin film was deemed poor due to the presence of additional SrVO<sub>3</sub> secondary peaks.

## **Introduction:**

A perovskite refers to any material with the crystal structure following the formula ABX<sub>3</sub> [1], and these perovskites are of great interest as result of the strange new properties that are exhibited like ferroelectricity, superconductivity, etc. [9]. For example, when LaAlO<sub>3</sub> is grown on SrTiO<sub>3</sub>, these two non-conductive materials display conductive behavior.

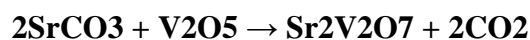
The word transparent conducting oxide (TCO) refers to electrically conductive materials that have high optical transmission at visible wavelengths. These materials are typically doped metal oxides and what makes them effective is the low resistivity and high transmittance properties that they have [1]. These transparent conducting oxides tend to be used in solar cells, displays, onto-electrical interfaces, etc. It is worth mentioning, that despite the extensive uses transparent conducting oxides have, they are fragile and break down with use.

Strontium vanadate is perovskite that has been the topic of research for condensed matter physics due to it being a strongly correlated material and having a low work function. SrVO<sub>3</sub> being a strongly correlated material, when SrVO<sub>3</sub> is doped or reduced in dimensionality, it undergoes metal-insulator transition [2,3,4]. Even more so, having been discovered that SrVO<sub>3</sub> has high transmittance and low resistivity, it has also been considered as a candidate as a transparent conducting oxide (TCO) this refers to materials used in screen displays or solar cells [1]. This is particularly important considering the industry standard, Indium Tin Oxide (ITO), is extremely limited in its amount and therefore, extremely expensive.

## **Procedure:**

### 2.1 Preparing the Target

Chemical reaction for Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub>:



The sample Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> was prepared first by using SrCO<sub>3</sub> and V<sub>2</sub>O<sub>5</sub> powders. For each of the starting materials, X-Ray Diffraction was done to ensure purity and to confirm the powders were not unknowingly contaminated, refer to Figure 1. Using the balanced equation, it was determined that to synthesize

approximately 1 gram of Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub>, 0.759 grams of SrCO<sub>3</sub> and 0.467 grams of V<sub>2</sub>O<sub>5</sub>. It should be noted that the balanced used to weight each of the reactants was not working properly resulting in a +/- 0.05 grams for each measurement. The stoichiometric amounts of the reactants were grounded using a motor and pestle until fine, the molar ratio being 2:1[6,7]. From there, the resulting mixture was transferred to an alumina crucible and heated to 1000 C for 24 hours in air in a furnace to calcine, ramping up to 1000 C in 4 hours and ramping down by letting the furnace naturally cool until it reaches room temperature. This was done to remove any carbon in the mixture. The powder pre-calcination was a yellow color, as seen in Figure 2, indicating a small band gap whereas the powder post-calcination was a blue-white color, as seen in Figure 3, indicating a large band gap, this is presumably due to vanadium.

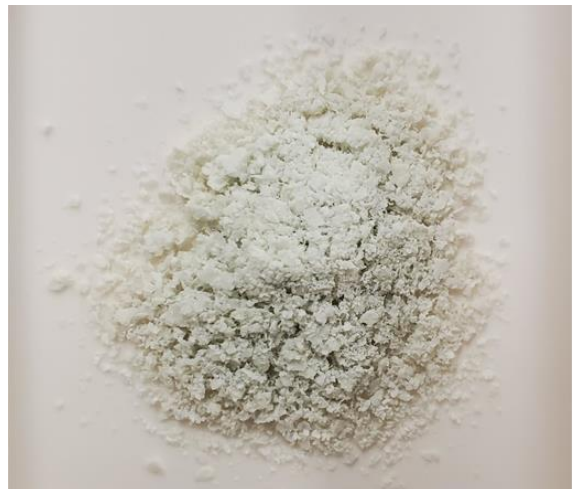
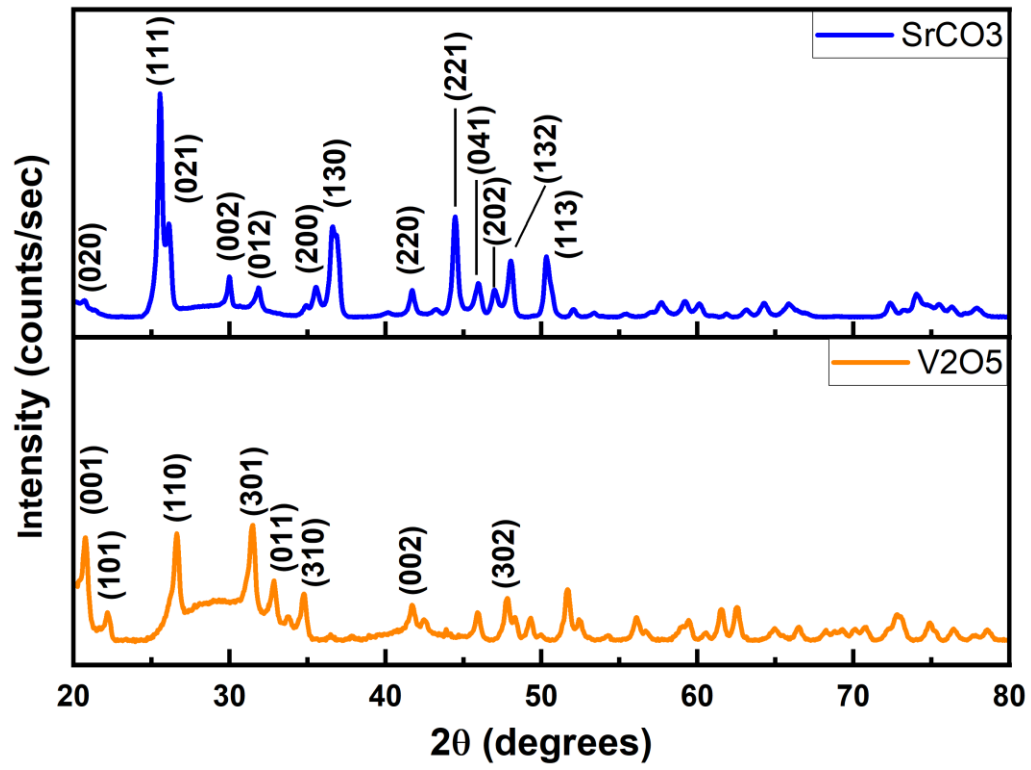
The process of regrinding and reheating the homogenously mixed powder was repeating until only Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> was present as observed through Powder X-Ray Diffraction (PXRD). In many other experiments where Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> was synthesized, the process was repeated, but in this experiment, it was found that repeating would be unnecessary despite the Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> powder still retaining the secondary phase Sr<sub>3</sub>V<sub>2</sub>O<sub>8</sub>. This additional phase was not concerning due to the presence of it being few and there having been other experiments conducted using 85 % SrVO<sub>3</sub> and 15 of a secondary phase [7]. While, there is a method to synthesize SrVO<sub>3</sub> from Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub>, in this experiment only Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> was synthesized and used as the target for Pulse Laser Deposition (PLD).

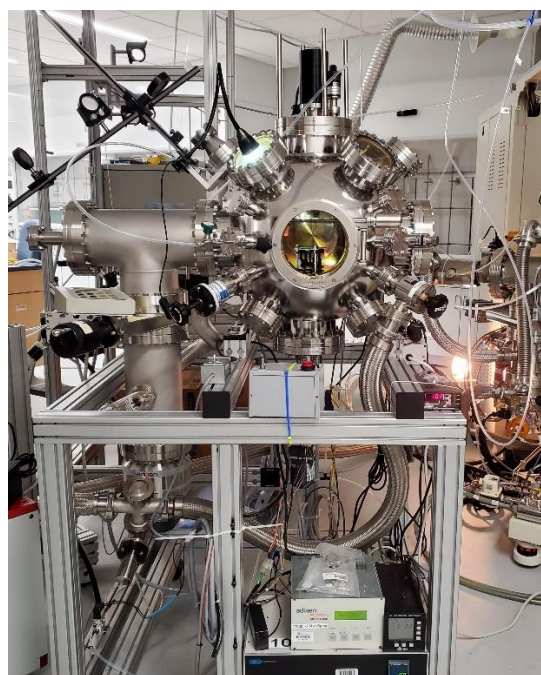
The steps are fairly similar, the only difference being that the SrVO<sub>3</sub> requires Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> to be heated in a furnace under gas flow of 95% Argon to 5% Hydrogen. SrVO<sub>3</sub> was not created in this experiment due to not having the gas and not having a working gas flowing furnace.

The calcinated powder was reground and was then molded into a 2mm diameter pellet using a dry pellet pressing die, as shown by Figure 4. The pellet die provided shapes the powder into a pellet, where it is then put under 21 tons of pressure using a hydraulic press, refer to Figure 5 for 1 hour. Once the pellet has been successfully formed, it is sintered at 1000 C for 24 hours using the same ramping up and down conditions as the calcination process. XRD should be performed on the sintered pellet to report any changes and determine if the pellet is still Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub>. Figure 6 shows the sintered pellet; the white peaks may indicate the powder may not have been ground enough.

## 2.2 X-Ray Diffraction (XRD)

XRD allows for us to determine the crystal structure, purity, and its current phase; for our experiment, this became extremely important due to SrVO<sub>3</sub> having several secondary phases like Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> and Sr<sub>3</sub>V<sub>2</sub>O<sub>8</sub>. One main concern for using Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> as the target for PLD was the crystal structure. Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> is triclinic meaning that each length of the crystal is unequal and the angles between them are also different making this crystal extremely unsymmetrical which results in the numerous peaks as seen in Figure 7. Whereas SrVO<sub>3</sub> has a cubic crystal structure, meaning each of the lengths are equal and the angles are all 90 degrees, which is what makes it symmetrical and have relatively fewer peaks compared to Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub>. Furthermore, having fewer, distinct peaks makes characterizing the XRD graphs simpler to observe if there are any additional secondary phases. Characterizing the XRD for Sr<sub>2</sub>V<sub>2</sub>O<sub>7</sub> was difficult due to the numerous peaks both of high and low intensity, especially since it was determined that the secondary phase Sr<sub>3</sub>V<sub>2</sub>O<sub>8</sub> peaks were also found. Sr<sub>3</sub>V<sub>2</sub>O<sub>8</sub> has a trigonal crystal structure meaning that





## References

- [1] R. Xu, et al. ACS Appl. Mater. Interfaces 12, 16462-16468 (2020)
- [2] G. Wang, et al. Phys. Rev. B 100, 155114 (2019)
- [3] M. Brahlek, et al. MRS Communications 7, 27-52 (2017)
- [4] M. Verma and R. Pentcheva, Phys. Rev. Research 4, 033013 (2022)

- [5] Y. Okada, et al. Phys. Rev. Lett. 119, 086801 (2017)
- [6] M. Onada, H. Ohta, H. Nagasawa, Solid State Commun. 79, 281-285 (1991)
- [7] T. Berry, et al. Journal of Crystal Growth 583, 126518 (2022)
- [8] J. G. Connell, et al. Appl. Phys Lett. 101, 251607 (2012)
- [9] J. Wang, G. Rijnders, G. Koster, Appl. Phys. Lett. 113, 223103 (2018)
- [10] T. Maekawa, K. Kurosaki, S. Yamanaka, Journal of Alloys and Compounds 426, 46-50 (2006)