Powder X-Ray Diffraction Data Analysis of $Sr_3Sn_2O_7$

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Introduction

The goal of this project is to study the data gathered from powder x-ray diffraction of the compound $Sr_3Sn_2O_7$. The data was collected in the Argonne National Laboratory in Illinois by using a powder form of the compound and compressing it in a diamond anvil cell with neon gas used as a pressure medium. A beam of monochromatic x-rays is then used to have the crystal structures reflect the beams. Due to the number of crystalline structures and their variance in orientation, we can safely assume that every 3-dimensional plane is producing a reflected beam, allowing us accurately to study the compound's changes at different pressures. 22 different pressures were studied, ranging from 1 gigapascal (GPa) to 24.0 GPa, and data was recorded from each pressure in crystallographic binary files, as well as a calibration file.

(a) (b)

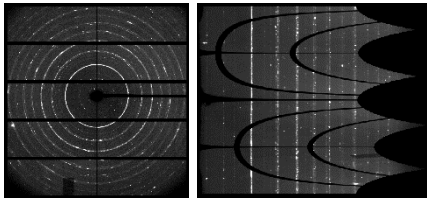

Figure 1. (a) Powder ring observed at Argonne National Laboratory. $Sn_3Sn_2O_7$ at 1 GPa. (b) Powder ring at of $Sr_3Sn_2O_7$ at 1 GPa with calibration

Data Analysis

The first step of the data analysis process was to go through each collected powder ring and mask any diffraction peaks appearing in the data set. These peaks usually appear in this data set due to the solidification of the neon gas we used as a pressure medium when recording our data. With the masked data, we then produce fits for our data using Rietveld refinement and Le Bail extraction methods to filter the background and produce values for the unit cell. As we increase the pressure, we expect to see a general decrease in each of the unit cell parameters at pressures where there is no phase transition as to represent the decrease in volume due to the extreme pressure imposed on the sample. At pressures where phase transitions occur, it is possible that some (but not all) unit values increase slightly, however the overall volume should continue to decrease (hence why not every unit cell parameter can increase during the same transition). We can predict when phase transitions might be occurring by watching for any new intensity peaks arising or previous peaks notably decreasing.

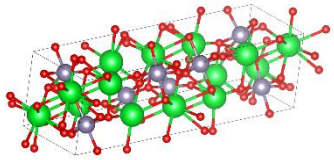

Figure 3. An A21am unit cell of $Sr_3Sn_2O_7$

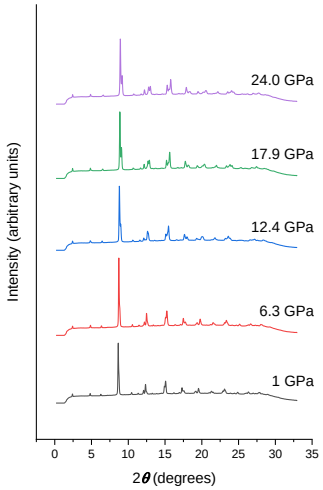

Figure 2. Relative intensity of the data gathered at 1 GPa, 6.3 GPa, 12.4 GPa, 17.9 GPa, and 24.0 GPa.

The unit cell is a representation of the smallest repeatable group of atoms in a crystal. As seen in Figure 3, each crystal structure also has a system and space group in which the symmetry of the unit cell is defined. In the case of $Sr_3Sn_2O_7$, the compound is an orthorhombic system with a space group of A21am, showing the symmetry of a crystal with equal angles of 90° but possibly unequal lattice parameters.

Discussion

As seen in Figure 2, the histogram of the gathered data shows the growth and shrinking of various peaks, most notably at about 8.5, 12.5, and 15.0 degrees. This change in intensity suggests the compound underwent phase transitions at some point during the data collection process

Next Steps

We are currently working towards either finding or creating crystallography information files that correctly represent the unit cell of the original compound and the phase transitions it undergoes at various pressures. With those files, we will be able to produce an accurate fit to the data.

References

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