

Misfit Layered Compounds

Misfit layered compounds are materials that have mismatched subsystems units cells thus, do not have alignment on all three crystallographic planes. Most misfit layered compound systems have similar **c** and **b** planes but have different **a** planes which are divided into **a_A** and **a_B**. The reason why this is important is that the **a_A** and **a_B** planes never line up which limits lattice vibrations throughout a system. Figure 1 shows these relationships.

Some examples of misfit layered compounds that are commonly researched in the Dave Johnson lab are:

- (MX)_a(TX)_b
- (TX)_a(TX)_b

M = Rare Earth; Pb, Sn, Bi, Sb,

X = Se, Te

T = Ti, V, Cr, Nb, Ta

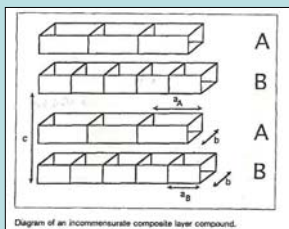


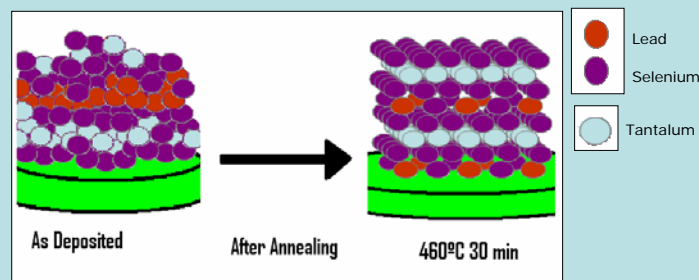
Figure 1: An example of the unit cell structure of a misfit layered compound.

Our hopes with our misfit layered system is to create a superconductive material with desirable thermoelectric properties.

Superlattice Growth and XRD

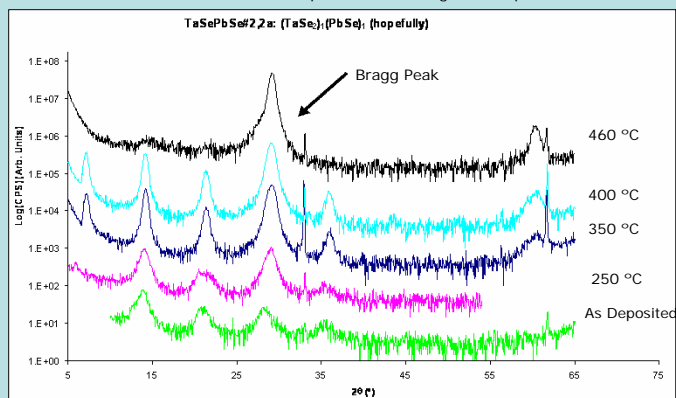
After depositing, the sample is mostly amorphous. To determine conditions for superlattice growth, an annealing study must be performed. Annealing, the process of heating a sample, creates order and crystallinity in the sample.

Figure 2: As deposited sample before and after annealing. Note the crystalline structure after introducing heat to the system.



X-ray diffraction is used to help characterize a sample. It uses x-ray beams directed towards a sample and detects the x-rays diffracted off the sample. The intensities can be used along with Bragg's Law, $2d\sin(\theta) = n\lambda$ to calculate the distance between layers, and the total thickness of a sample. (See Analyzing and Calculating Data for more information.)

Figure 3: Annealing study conducted on TaSePbSe #2, a 1 to 1 layer ratio. Note as the temperature increases, the intensity of the peaks increase all except for the 460°C scan where it was concluded that the sample was oxidized and most of the selenium evaporated off ruining our composition.



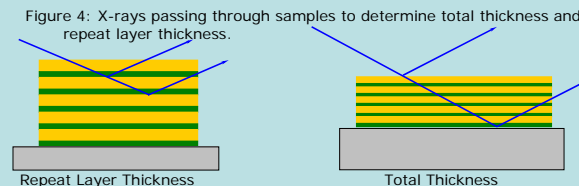
Analyzing and Calculating Data

Using Bragg's Law, you can calculate the repeat layer thickness, and the total thickness of your sample. Using the Kiessig fringes found on low angle scans total thickness of a sample is calculated. The Kiessig fringes are the constructive interference of the x-ray beam from a front to back reflection of the x-ray beam. Repeat layer thickness is calculated by the Bragg peaks and tells you the thickness of a layer. As the x-rays diffract from different layers, the intensity of the diffracted beam increases due when the diffracting planes are well aligned (see Figure 4).

$$\text{Bragg's Law: } 2d\sin(\theta) = n\lambda$$

$$d = \text{distance} \quad \theta = \text{Angle of Incidence}$$

$$n = \text{random whole number integer} \quad \lambda = \text{X-ray Wavelength}$$

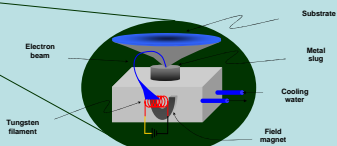
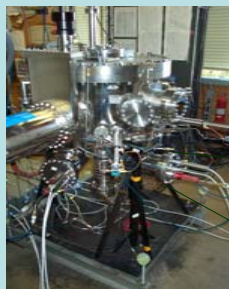


Deposition Chamber

The deposition chamber is the tool used to create our samples.

Under high vacuum, metals are deposited by an electron beam gun to our substrate. Selenium is deposited with an effusion cell instead. The deposited material from an electron beam gun is controlled by an electron beam current.

Computer controlled shutters control the amount of time a sample is deposited upon. By closing and opening, one can control the amount that is deposited on a substrate. This is monitored by the crystal monitors which keep track of deposition thickness. Quartz vibrates at a well known frequency. When other materials are deposited on quartz the fundamental frequency of vibration is shifted. The amount of material deposited is found by applying the density and Z-ratio of the deposited material to a thickness calculation.



Conclusion

We found that the intensities of the Bragg peaks increased as the annealing study was carried out indicating that the samples were becoming more crystallized. When there are more layers of TaSe, there are more Bragg peaks evident in the X-ray data. The exact nature of this trend is, as yet, undetermined. More samples with different layer combinations must be produced.

Future Directions

In the next few weeks, we hope to continue to make samples and conduct annealing studies on them. Once we understand how to make a wide variety of samples, we will find the layer ratio that gives us the best thermoelectric properties.

References

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