Dielectric Functions of $(Bi_xIn_{1-x})_2Se_3$ Films Grown on Sapphire Substrates

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Abstract

Analyzing a series of in-situ ellipsometry spectra of MBE-grown $(Bi_xIn_{1-x})_2Se_3$ films grown on sapphire substrates, we have explored how their dielectric functions varies with alloy concentration. Starting with the nominal thicknesses determined by RHEED, we fit both the thickness and the dielectric function of each film. The sapphire substrate was modelled with birefringent optical constants. The dielectric functions of $(Bi_xIn_{1-x})_2Se_3$ films were modelled using several Kramers-Kronig consistent oscillators. Upon further analysis, we have deduced how some of the main oscillator-parameters change with alloy concentration, which will be important if $(Bi_xIn_{1-x})_2Se_3$ alloys are to be used in optoelectronic applications. function of both alloy concentration and temperature.

Introduction to Material

Topological insulators have conducting properties on their surface while their bulk is insulating. This is demonstrated in the band structure on the right where the green lines show the surface conduction property. The arrows on the green lines indicate protected surface spin states which also make this material unique.

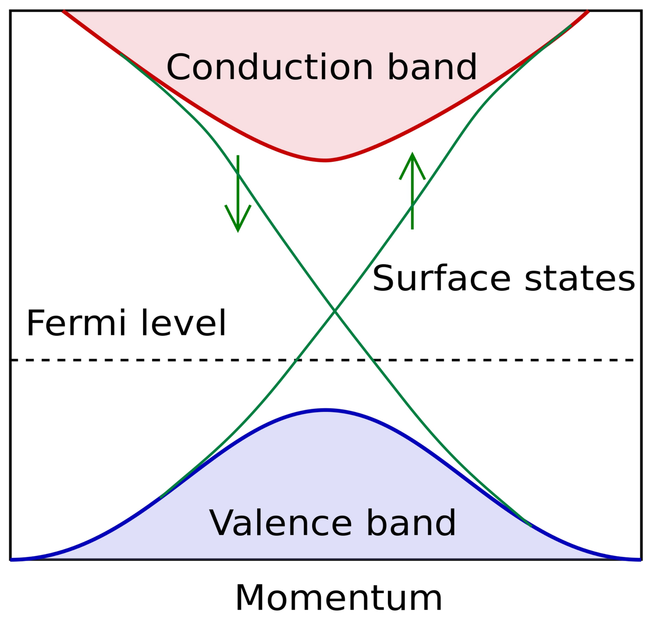


Figure 1: Band structure of Topological Insulator [1]

7 Topological Insulator Samples Studied:

- Bi_2Se_3 (100%)
- In_2Se_3 (0%)
- 5 alloys: $(Bi_xIn_{(1-x)})_2Se_3$
  Approximate percentage Selenium for each alloy: 90%, 80%, 60%, 50%, 25%

Theory

Spectroscopic Ellipsometry is a technique in which linearly polarized light of a single wavelength is reflected off of a sample and the reflected polarization and intensity is recorded. This information is interpreted into two quantities, ψ and Δ. The ψ corresponds more to the relative intensity between the two polarized light waves, while Δ corresponds to the relative phase difference. The equation that governs this relationship is given as follows:

$$\frac{R_p}{R_s} = \tan(\psi)e^{i\Delta}$$

In this case, R_p and R_s are the total reflection coefficients with respect to the p and s polarizations. Both R_p and R_s are complex numbers which are related to the dielectric function and thickness of the sample that is monitored via ellipsometry.

Theory cont.

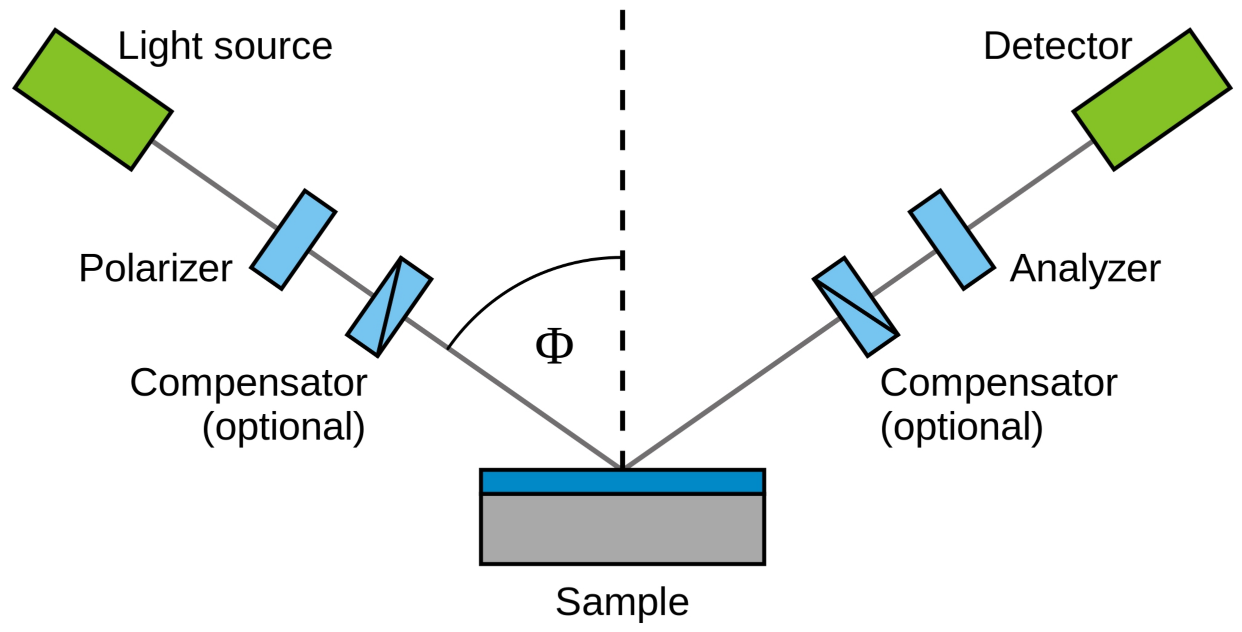
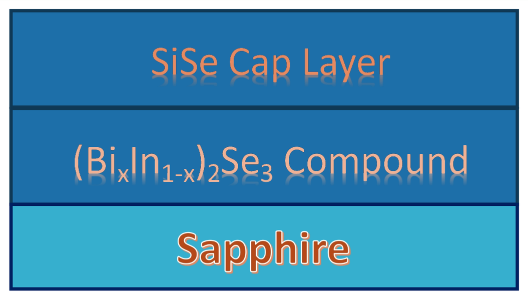


Figure 2: Overview of spectroscopic ellipsometry [2]

Modelling Ellipsometry Data



Firstly, 1mm of sapphire was prepared as substrate. Then, a layer of 30QL $(Bi_xIn_{1-x})_2Se_3$ compound was grown on top of the substrate at 225 C°. After being cooled down to room temperature, a cap layer of about 20nm was formed to prevent the compound from direct exposure to the atmosphere.

Figure 3: Structure of the compound samples

All of the experimental data were taken at room temperature (10C°) at a scan angle of 73.6° after preparation of the samples. Each sample was modelled layer by layer. Take one of them as example:

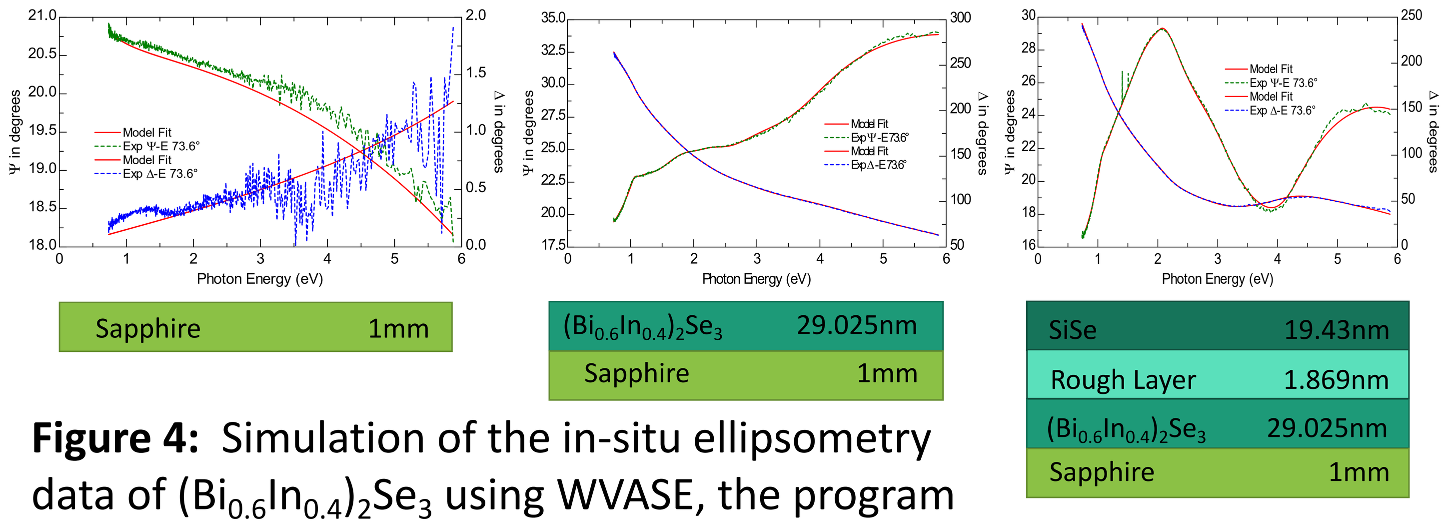


Figure 4: Simulation of the in-situ ellipsometry data of $(Bi_{0.6}In_{0.4})_2Se_3$ using WVASE, the program designed to fit ellipsometry data.

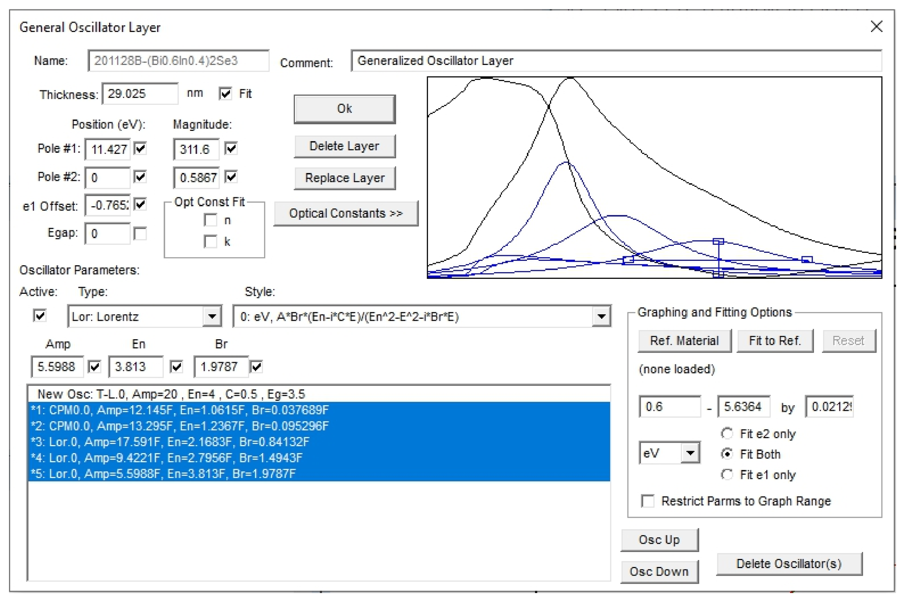
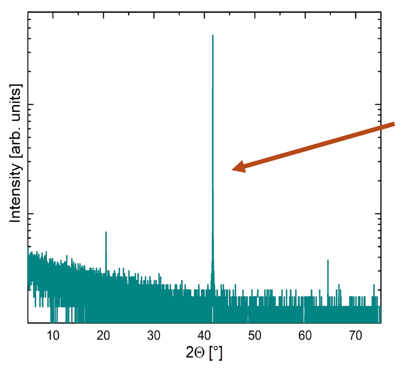


Figure 5: Oscillators used to simulate the dielectric function

As shown in figure 4, the main idea is to simulate ψ and Δ of each step with general oscillators which are mathematical models describing the energy bands. Note that ψ and Δ are closely related to the reflectivity which is a function of the dielectric functions.

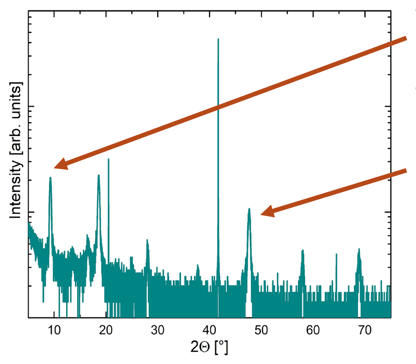
The Critical Point Models (CPM) and the Lorentz Oscillators are two of the classical models for semiconductors. Each of them contributes to the total dielectric function as shown by the blue bumps.

It is worth mentioning that X-Ray diffraction data were acquired after growth of the cap layer in order to examine quality of the crystalline for each of the samples. A sample with only sapphire and the SiSe was prepared in order to identification its diffraction peaks.



The 3 diffraction peaks come from the sapphire substrate. SiSe doesn't maintain a crystal structure and thereby doesn't generate X-ray diffraction peaks.

Figure 6: X-ray diffraction scan of the calibration sample (Sapphire+SiSe)



The 6 peaks are from the compound layer. The three on the right of the sharp central peak represent the same crystal structure as the three on the left, just with higher order Miller indices.

Figure 7: X-ray diffraction scan of the $(Bi_{0.6}In_{0.4})_2Se_3$ sample

Results

(1) The dielectric function of an alloy changes correspondingly to the proportion of its components. Although dielectric function also varies with the thickness (when it is below 20nm) and temperature, influences from the two factors are negligible, because temperature and thickness are fairly still for our samples.

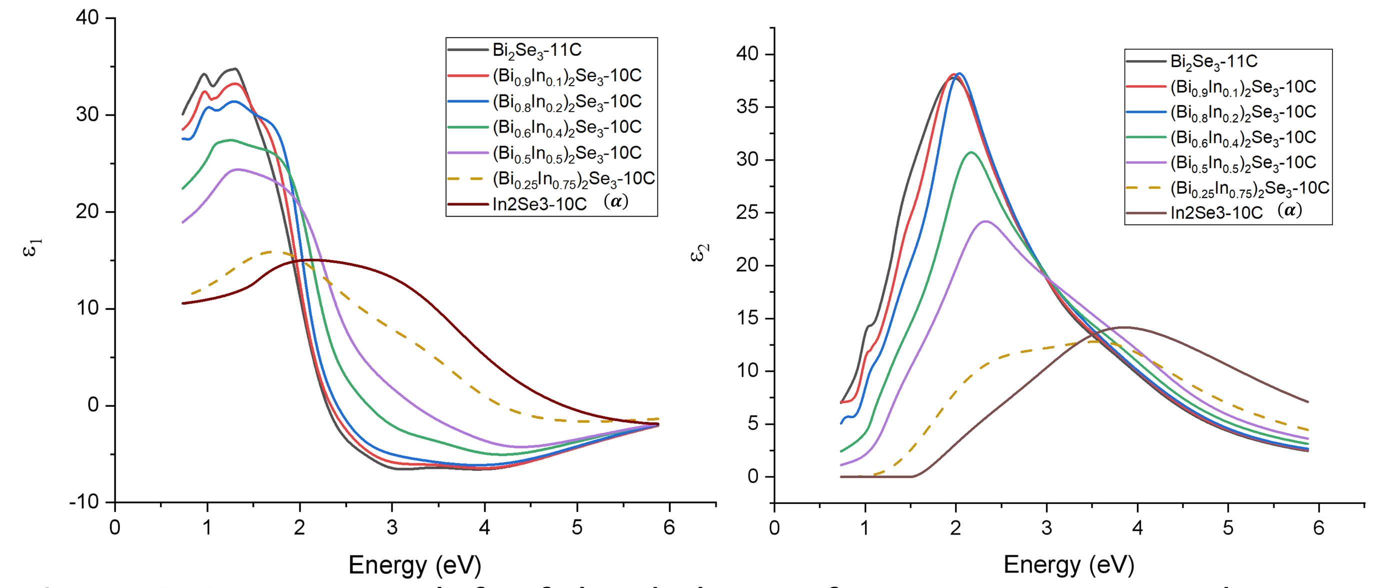
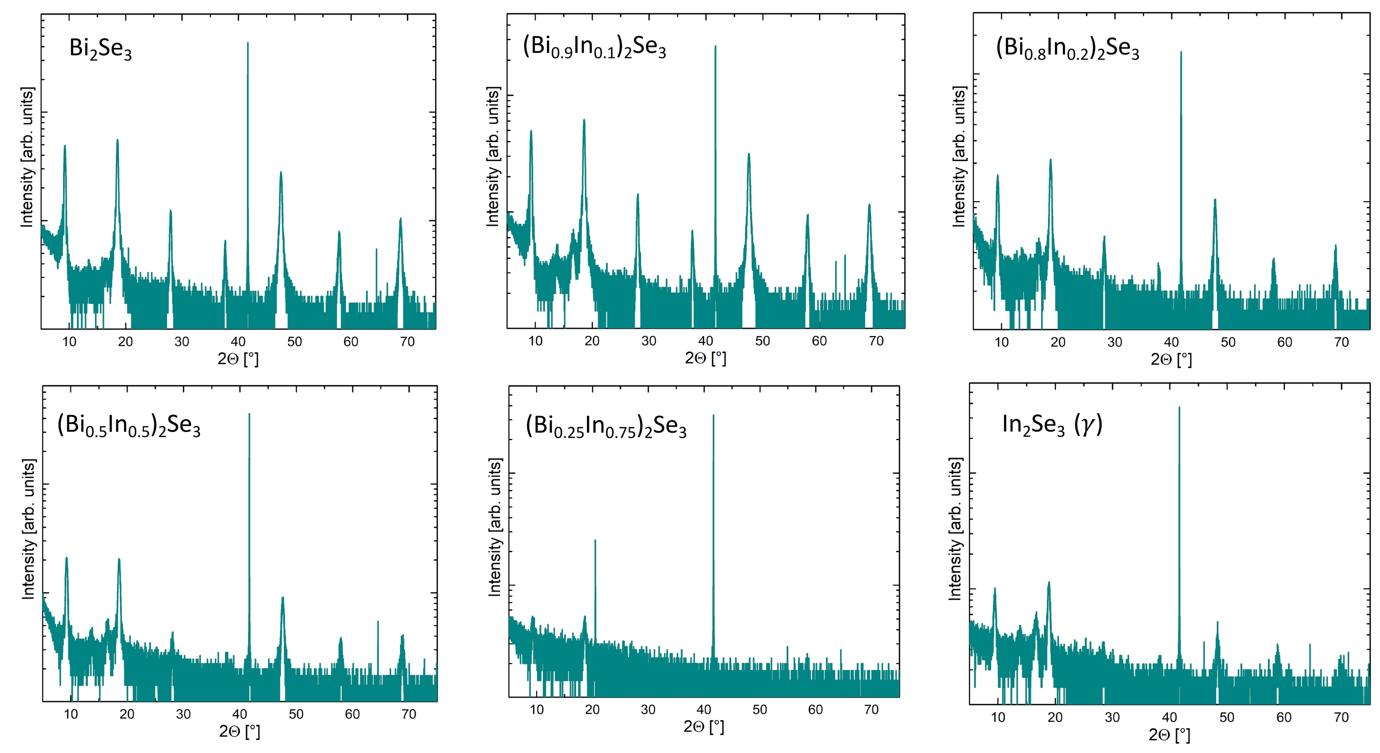


Figure 8: Systematic shift of the dielectric functions corresponding to percentage of Bismuth

(2) By examining the X-ray diffraction patterns, we found that qualities of the crystal structures rely on proportion of Bismuth in the compound. Quality of the crystalline decreases when proportion of Bismuth reduces. When the amount of In_2Se_3 surpasses 50%, the crystal structure becomes poor. This result suggests that Bismuth Selenide grow better on the sapphire substrate than Indium Selenide. In fact, Bi_2Se_3 is able to recover from the lattice mismatch while In_2Se_3 usually fails to do so. This explains why the $(Bi_{0.25}In_{0.75})_2Se_3$ sample doesn't match the trend of transition.



(3) In_2Se_3 seem to grow different phases on different substrates. For example, it forms a hexagonal crystal structure (γ −phase) on sapphire substrate, and a rhombohedral crystal structure (α −phase) on Bismuth Selenide. Comparatively, In_2Se_3 grows the best on Bi_2Se_3.

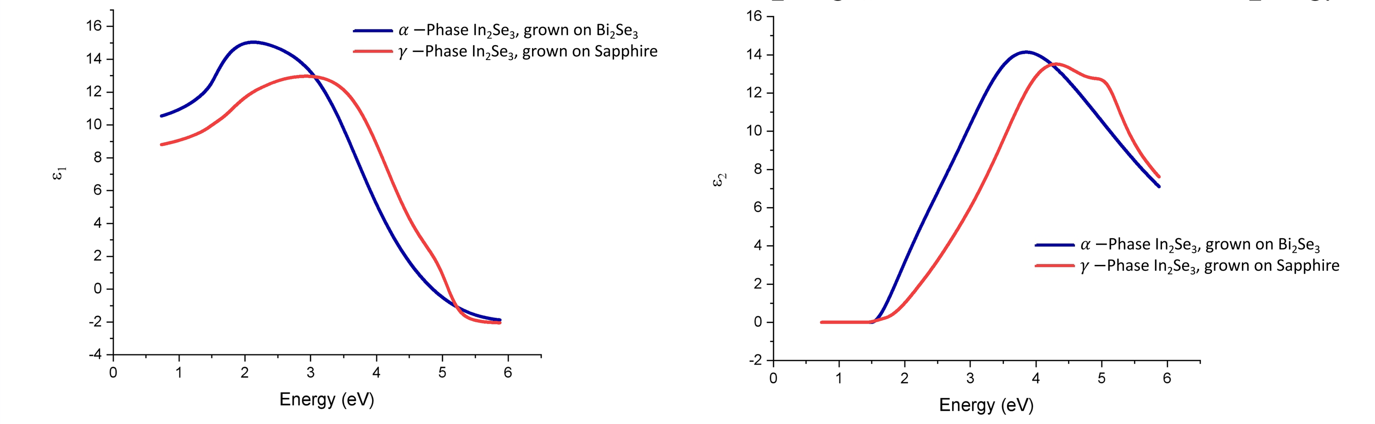


Figure 9: Comparison of the two phases of In_2Se_3

References

[1]https://upload.wikimedia.org/wikipedia/commons/thumb/f/fd/Topological_insulator_band_structure.svg/2000px-Topological_insulator_band_structure.svg.png
[2]https://upload.wikimedia.org/wikipedia/commons/thumb/2/27/Ellipsometry_setup.svg/2000px-Ellipsometry_setup.svg.png

Acknowledgements

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