Temperature Dependent Dielectric Functions of Topological Insulators

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Abstract

Topological insulators (TI) are semiconductors with a special property which allows them to conduct charge on their thin surfaces (~5-10 nm) while having an insulating phase in their bulk. In this work, we studied a series of topological insulators (i.e., Bi_2Te_3, Bi_2Se_3 and their alloys) that were grown on top of GaAs substrates using molecular beam epitaxy. The samples were scanned using spectroscopic ellipsometry between 200 nm and 1600 nm. In order to determine the temperature dependent properties, we recorded scans from 22 K to 300 K using a liquid-helium-cooled cryostat. The experimental spectra were modelled to obtain the dielectric functions of the topological insulators. Specifically, we used a free-electron oscillator, called a Drude oscillator, to model the conduction of the surface layer of the topological insulator. Additionally, another oscillator was included to model the band gap properties of the bulk layer. By tracking the parameters of the two oscillators, we were able to deduce how the electrical conductivity, and the band gap properties evolve as a function of both alloy concentration and temperature.

Introduction to Material

Topological insulators conduct on their surface while insulating in their bulk. 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.

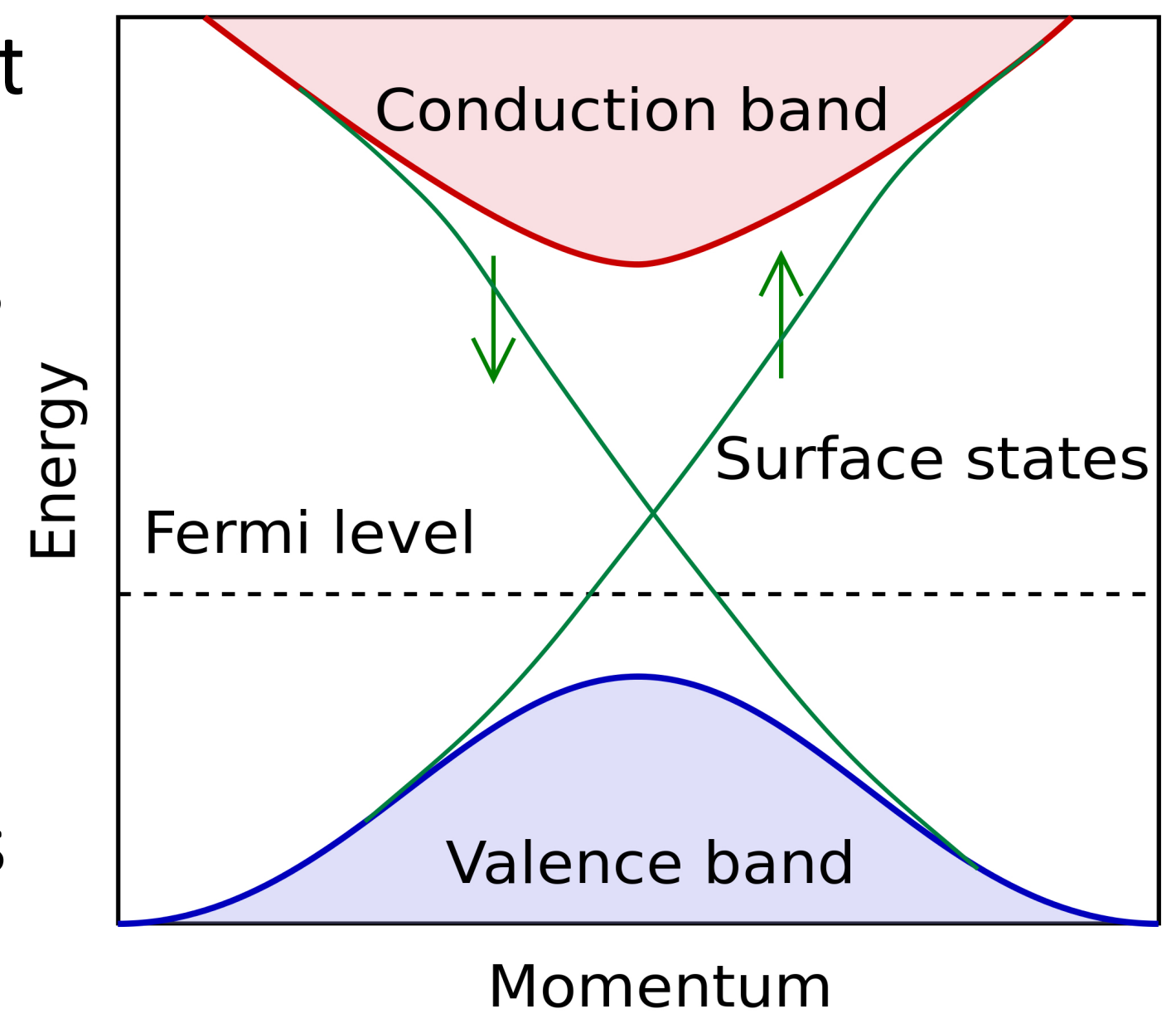


Figure 1: Band structure of Topological Insulator [1]

7 Topological Insulator Samples Studied:

- Bi_2Te_3
- Bi_2Se_3
- 5 alloys: $Bi_2(SeTe)_3$

Approximate percentage Selenium for each alloy:
30%, 45%, 50%, 63%, 93%

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.

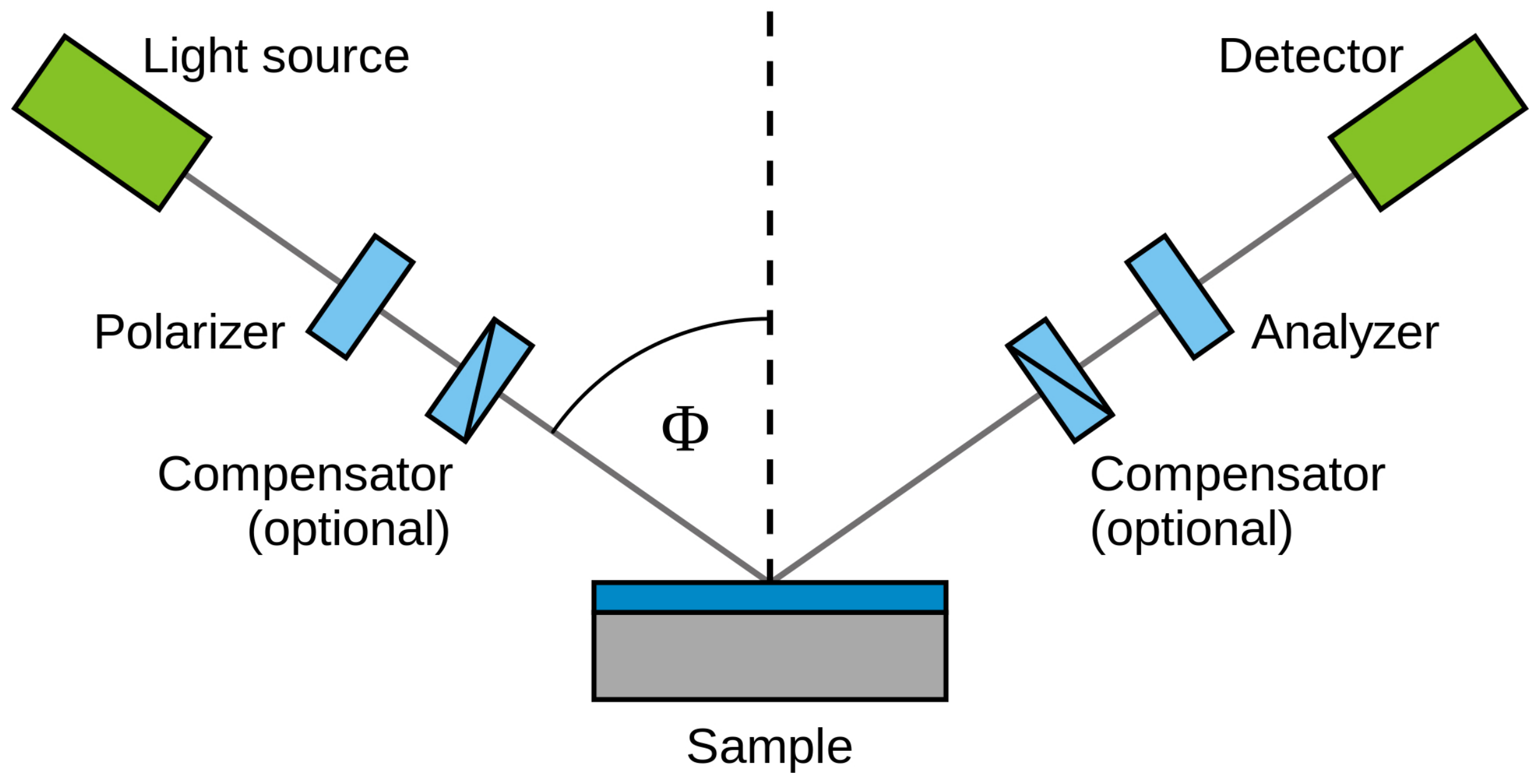


Figure 2: Overview of spectroscopic ellipsometry [2]

Experimental Details

For each sample, we followed a data collection procedure:

- Place sample in cryostat under vacuum
- Heat to remove protective Selenium layer from the sample
- Use Liquid Helium to take Temperature dependent Spectroscopic Ellipsometry scans at 20K, 66K, 100K, 150K, 200K, 300K
- Model these scans in order to determine the Temperature Dependent Dielectric Functions

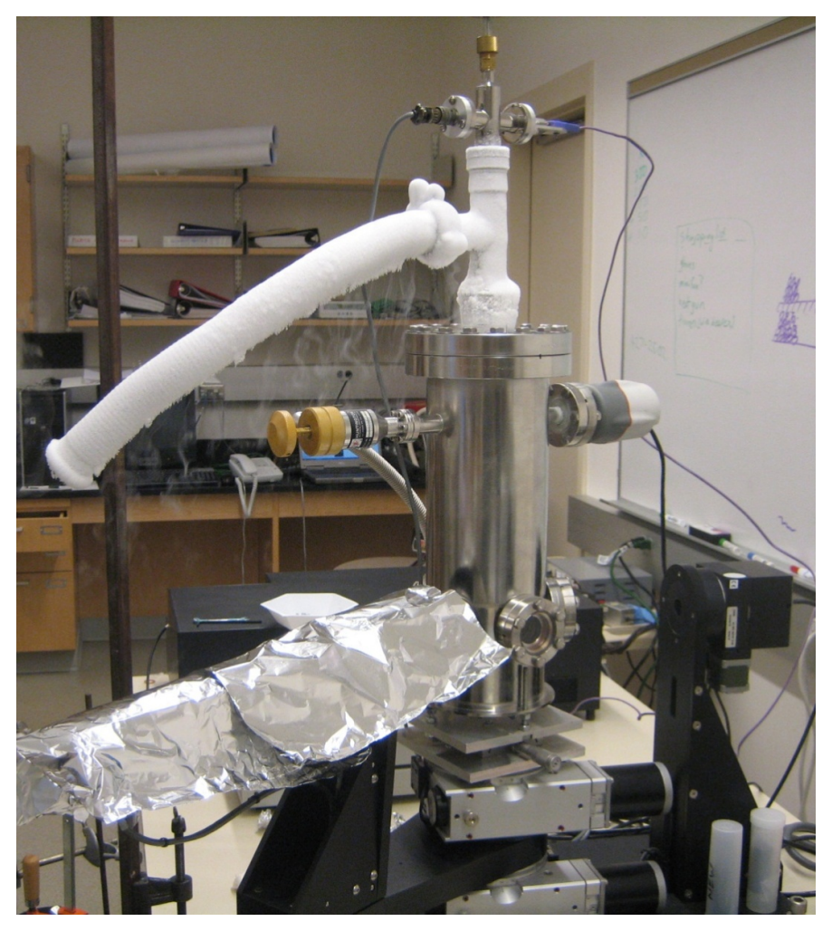


Figure 3: Cryostat used to perform low-temperature measurements

Selenium Cap Removal

Each sample comes with a layer of Selenium to keep it from oxidizing and corrupting the surface. This cap has a lower boiling point than the sample and its substrate. Hence, to remove the cap, we heat it in vacuum for 10 minutes, monitoring the intensity of the light reflected by the sample. The sudden increase in intensity suggests, the evaporation of the cap-layer.

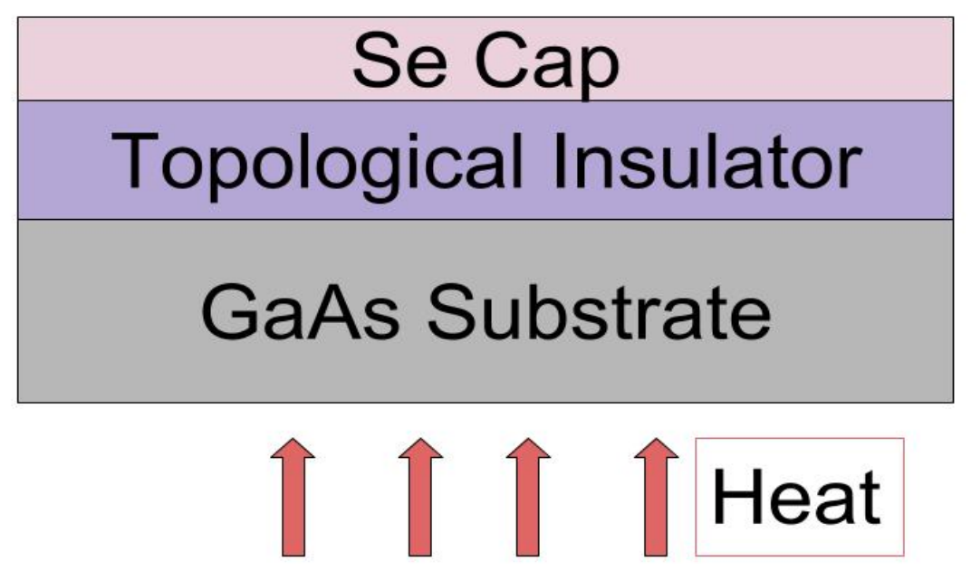
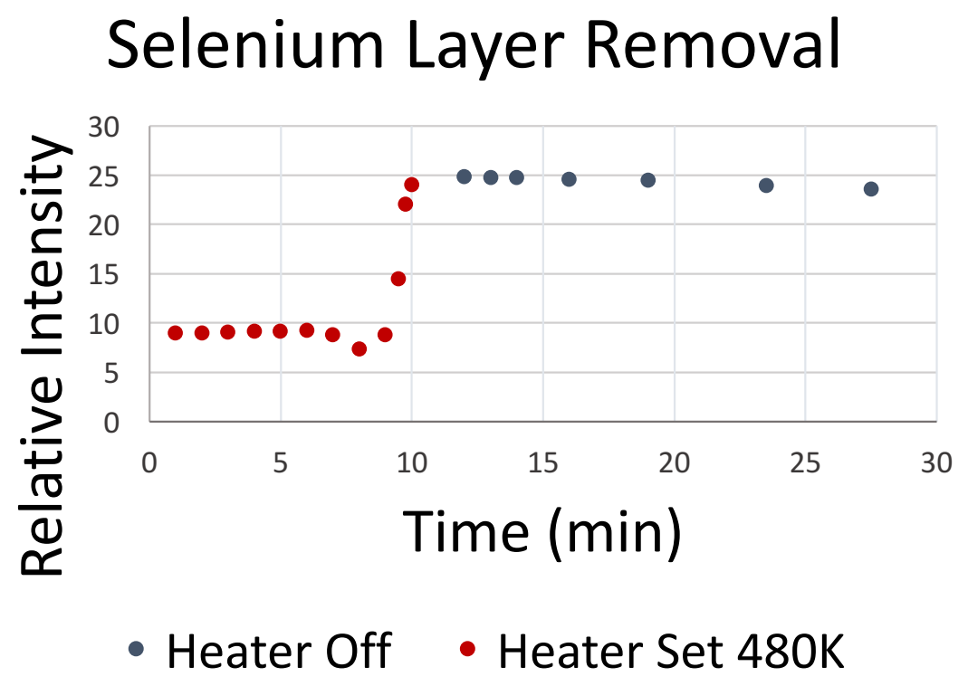


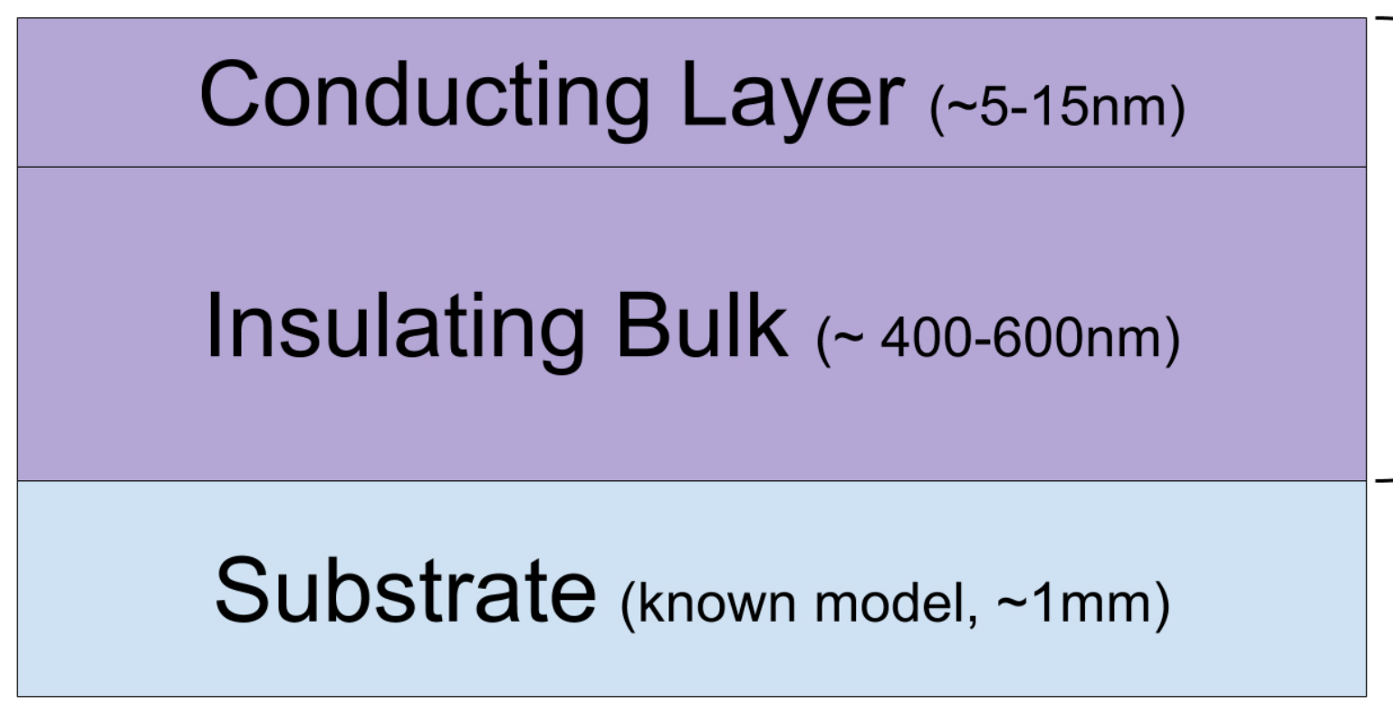
Figure 4: Cross-section of sample, not to scale



Right, Figure 5: Intensity vs Time for Selenium Layer Removal Process

Modelling Ellipsometry Data

Overview of modelling



Topological Insulator:

- 1 layer models model behavior of bulk and upper layer together
- 2 layer models separate conducting behavior from the bulk

Each sample was modelled in three ways;

- One layer isotropic oscillator model
- One layer anisotropic oscillator model
- Two oscillator layers, lower layer anisotropic model

Results

Oscillators

Each model uses two oscillators:

- Drude models absorption of free electrons related to the conducting surface.
- CPM0 models the materials bulk band gap properties

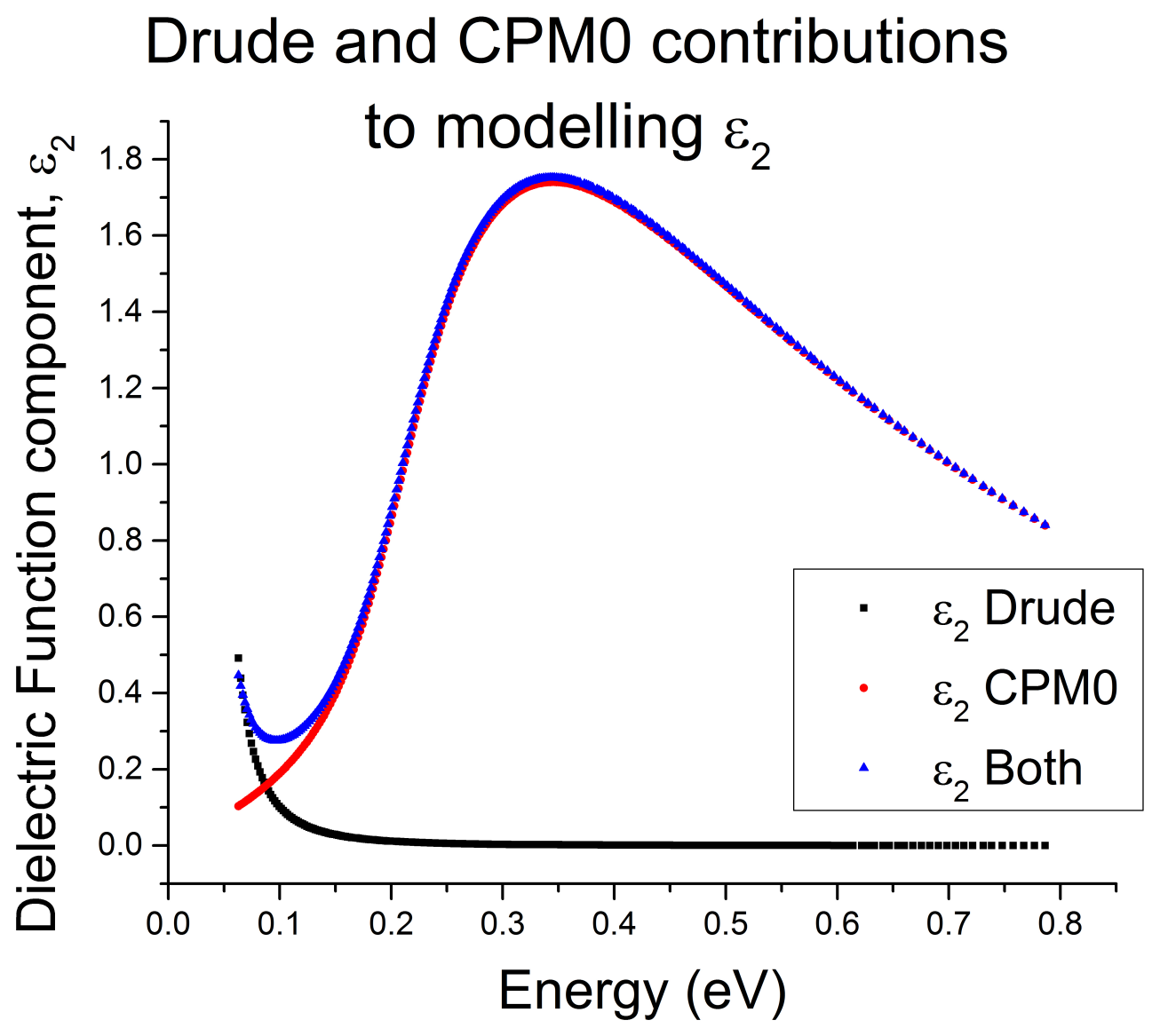


Figure 6: Oscillator Contributions to Dielectric component, ϵ_2

For each set of ellipsometry data, we applied all three models independently. When a mathematical model fits well, we can use the parameters of the model to infer information about physical properties of the sample. The figure on the right shows modelled data.

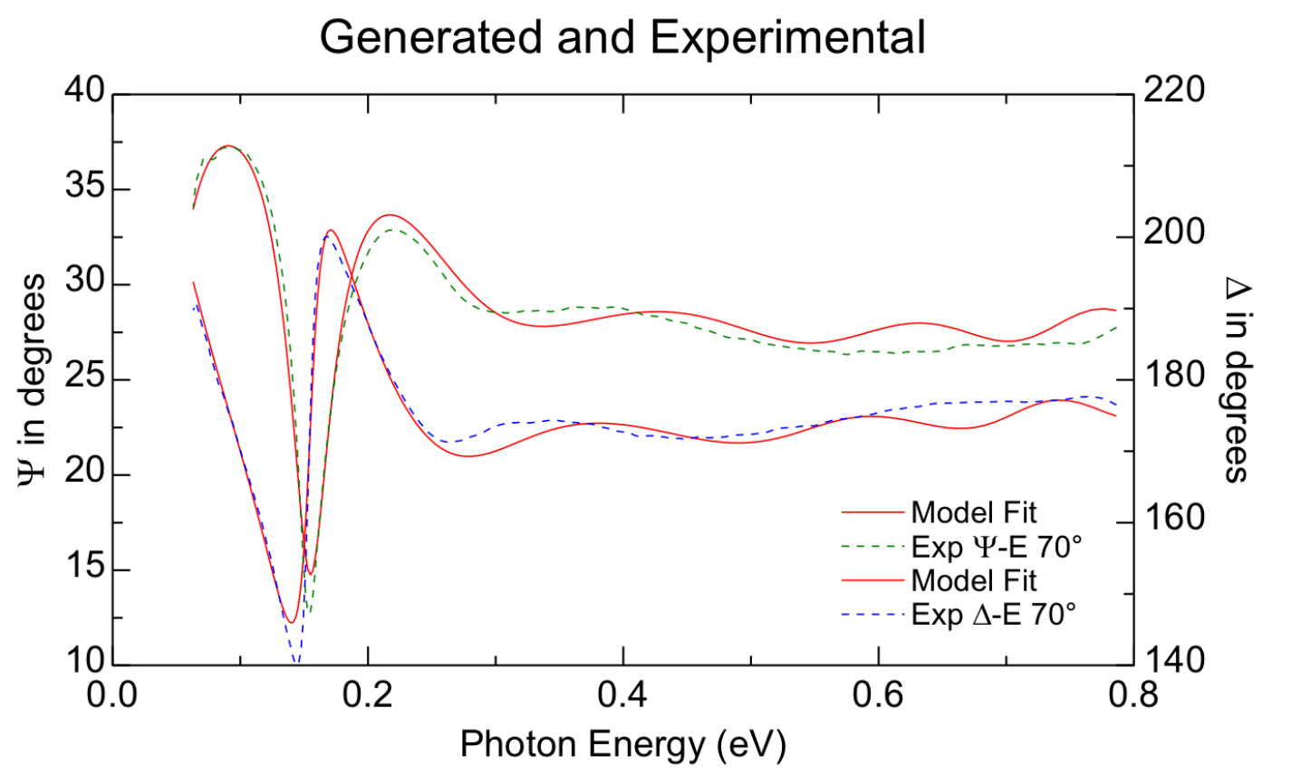


Figure 7: Raw data (green & blue) and the model-fit (red).

Isotropic vs anisotropic

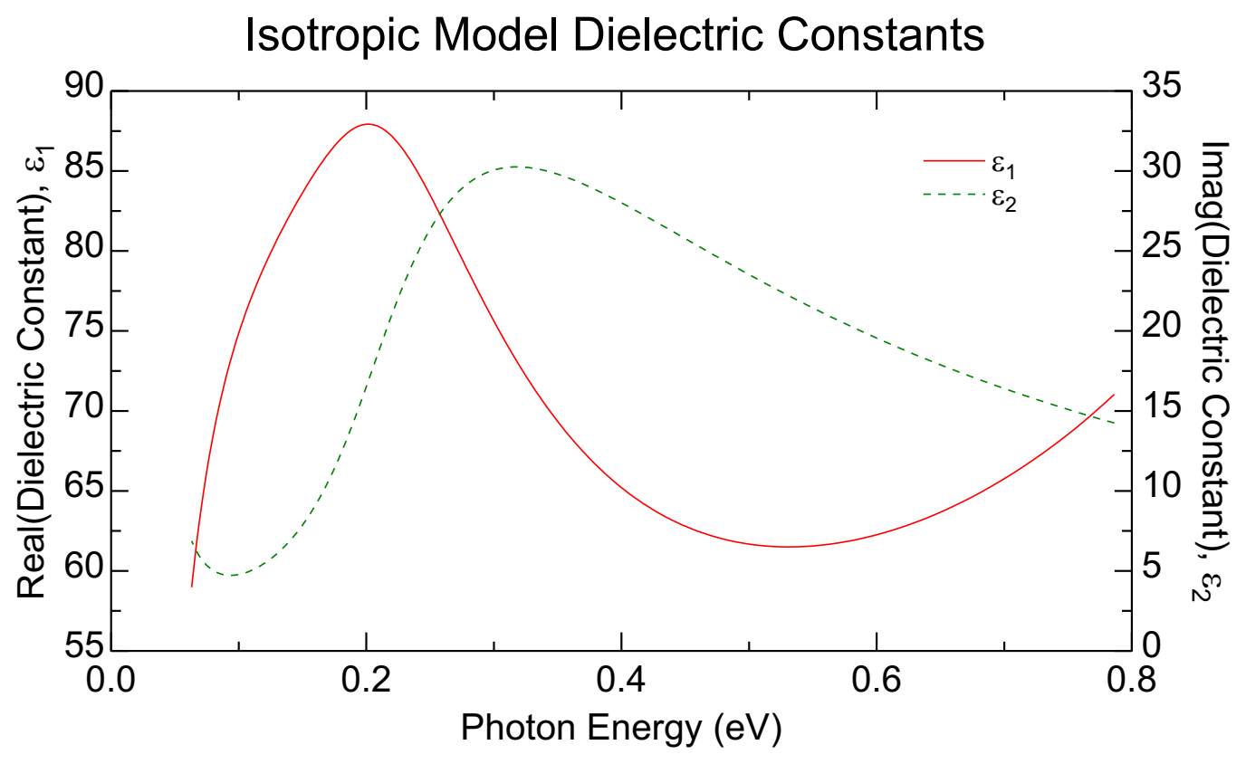


Figure 8: Isotropic modelled dielectric function for Bi_2Te_3

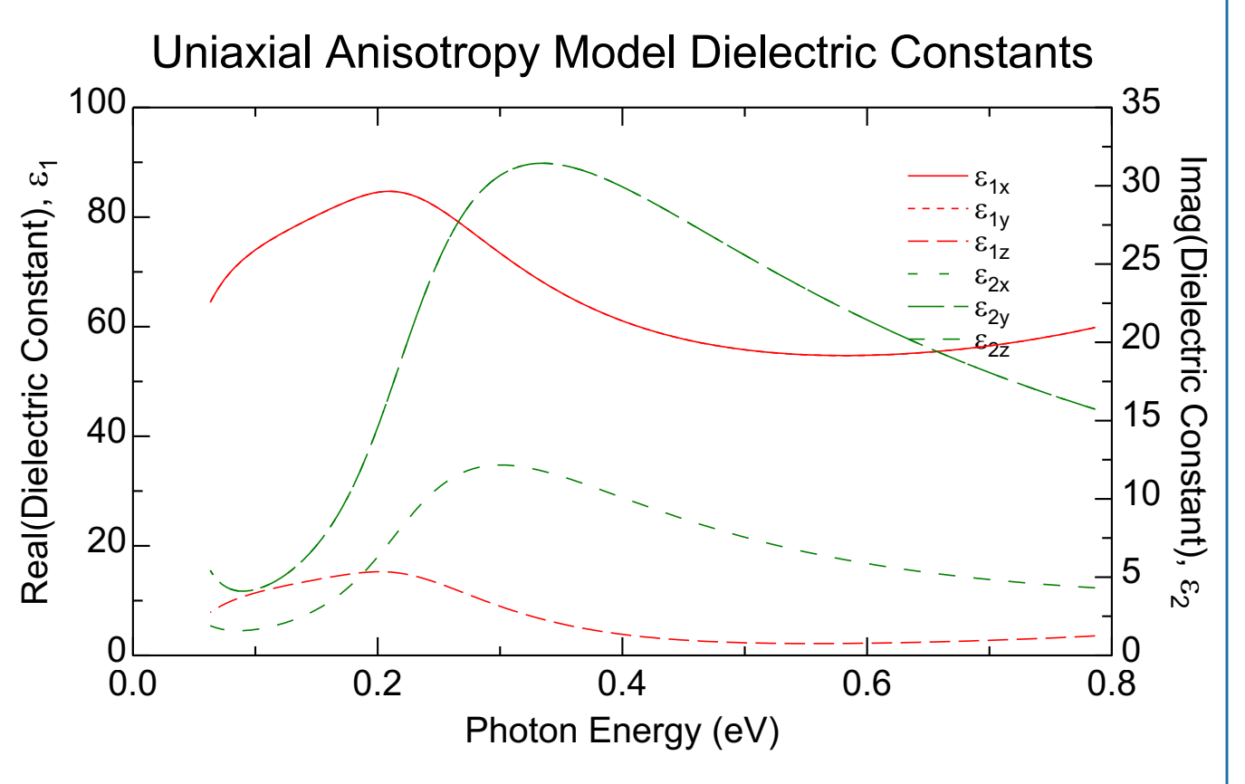


Figure 9: Single Layer Anisotropic modelled dielectric function for Bi_2Te_3

Generally, Uniaxial Anisotropy improved fits by 10-30%.

Temperature Dependence

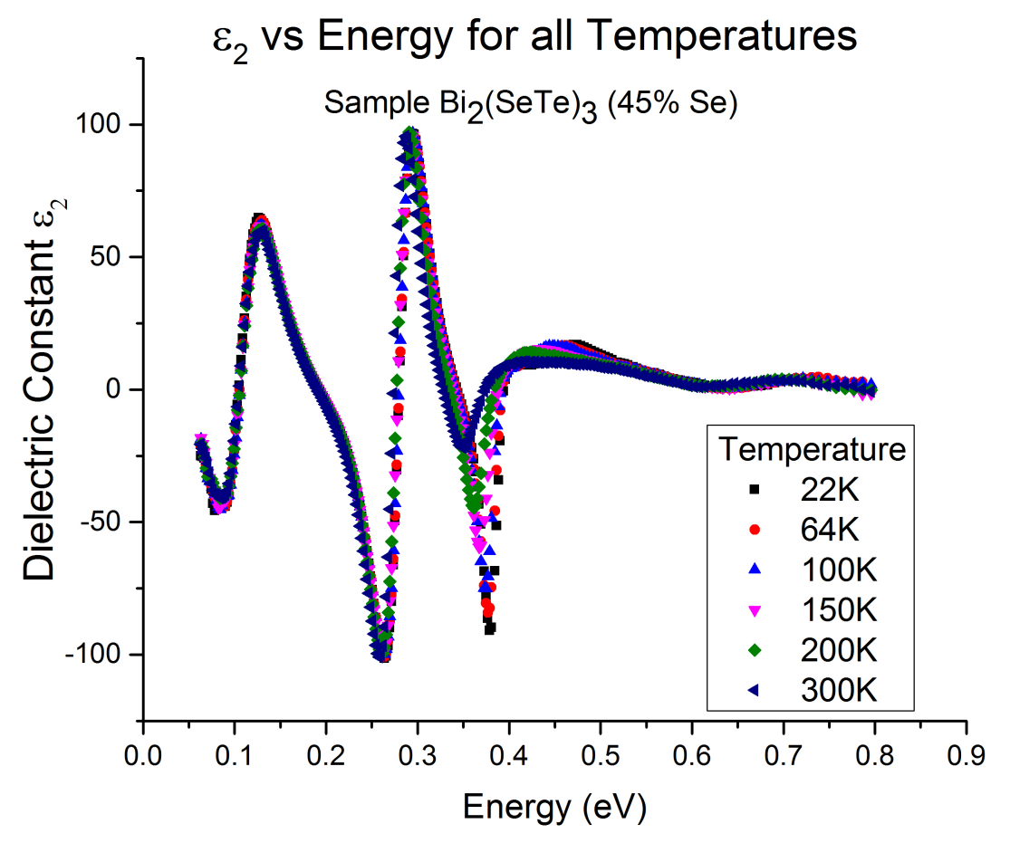


Figure 10: ϵ_2 vs Energy for a sample at six different Temperatures

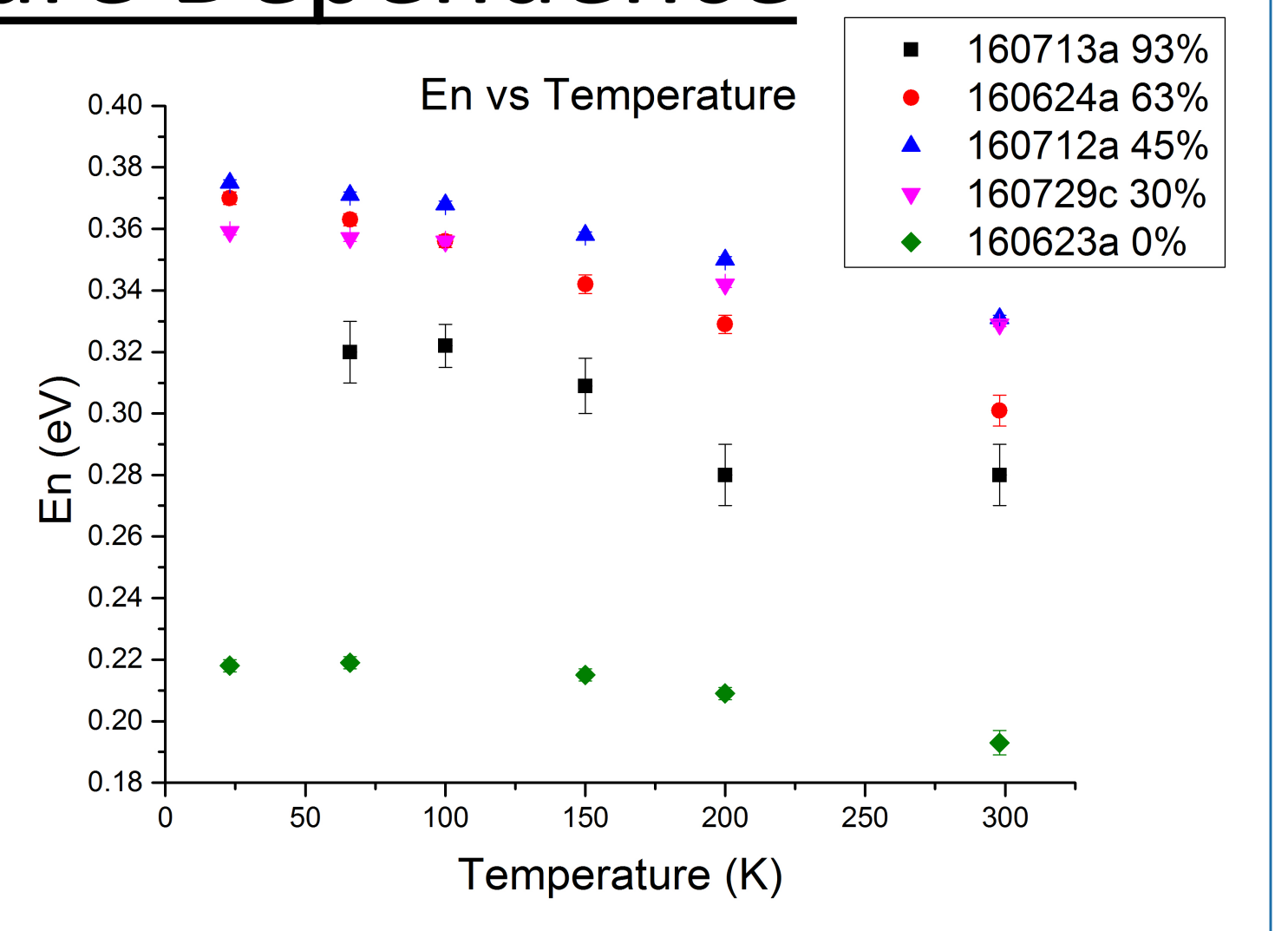


Figure 11: En vs Temperature for five samples. En is an oscillator parameter related to the band gap energy

References and Acknowledgements

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[2] Buntgarn, at the English Wikipedia project [CC-BY-SA-3.0 (http://creativecommons.org/licenses/by-sa/3.0/)], via Wikimedia Commons

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