Growth of Bi_2Se_3 Single Crystals Using an Optical Floating Zone Furnace

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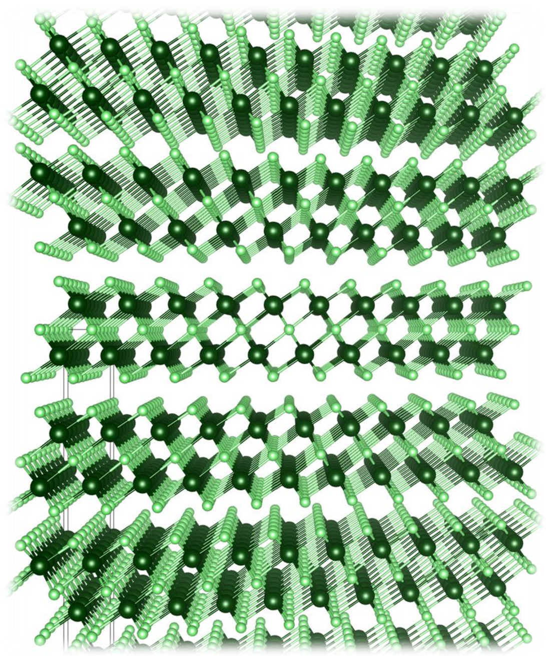
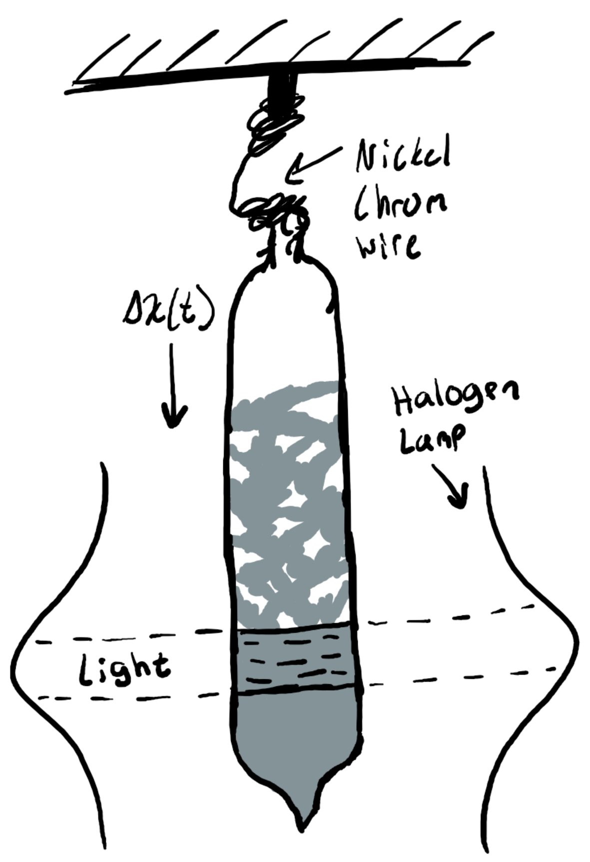
Introduction & Background

Single Crystals: Single crystals are materials where the atoms are arranged in a perfect periodic pattern throughout the entire material. In the picture to the right, there is a clear pattern of Bi and Se atoms showing the material is a single crystal. They can be grown naturally in the earth or can be created in a lab through various methods.



Bi_2Se_3 Crystal Structure

Optical Floating Zone Furnace: One crystal growth method uses an optical floating zone furnace. This furnace uses halogen lamps to focus light onto a specific area of a material, reaching a maximum temperature of 2000°C! The light can move up and down the material to melt precise locations. This allows the furnace to melt the material from bottom to top, slowly creating a single crystal.



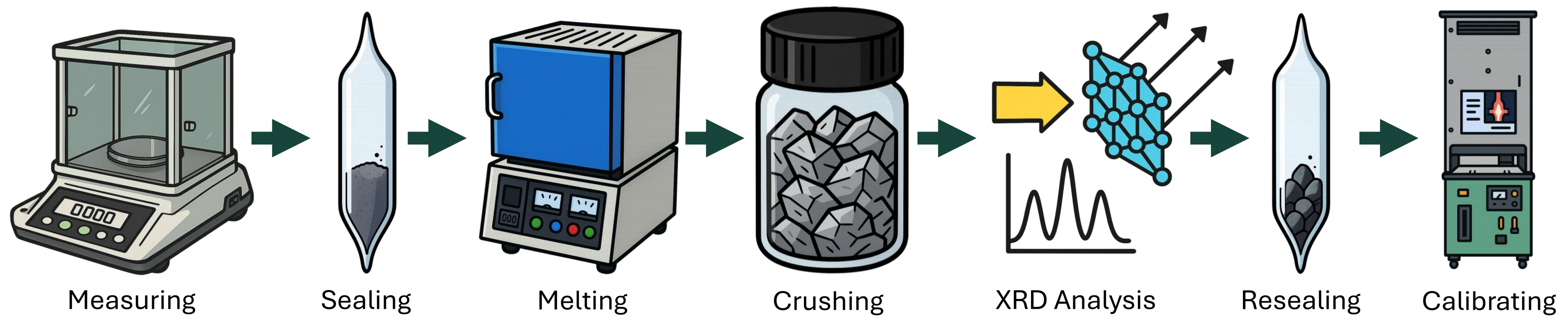
Optical Floating Zone Furnace Setup

Inside Optical Floating Zone Furnace

Importance in Electronics: In electronics and materials science, single crystals are extremely valuable because they allow electricity to flow smoothly and efficiently. Material imperfections such as point defects or green boundaries. can block or scatter electrons, reducing the material's electrical conductivity. Single-crystal materials are commonly used to make semiconductors, solar cells, and thermoelectric devices.

Project goal: My goal with this project was to use an optical floating zone furnace for the growth of Bi_2Se_3 single crystals, which is a material that is interesting for thermoelectric applications.

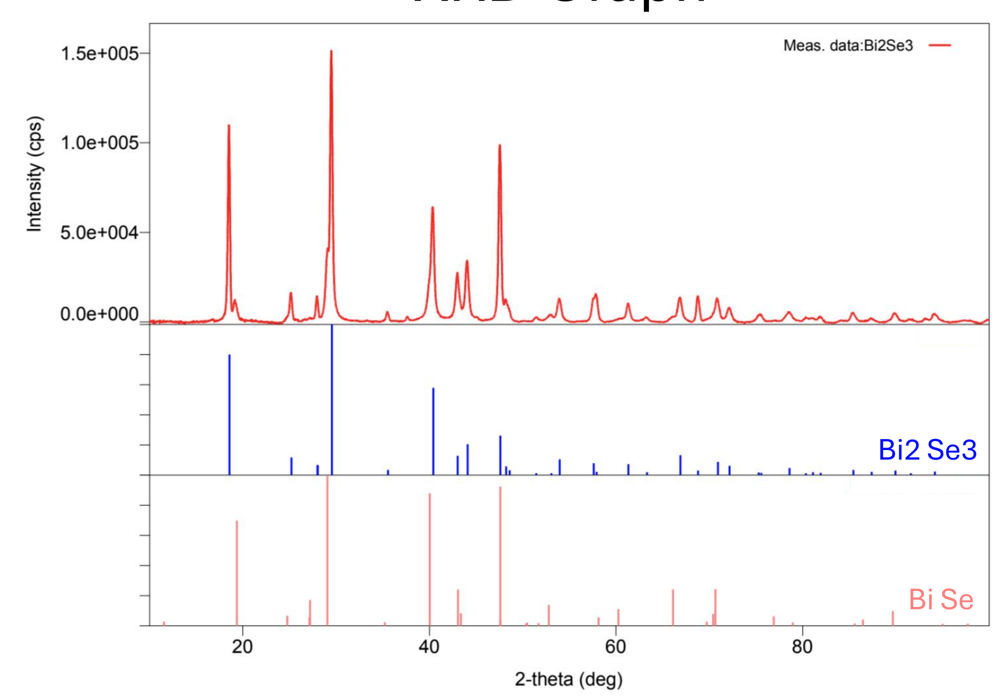
Preliminary Growth Results



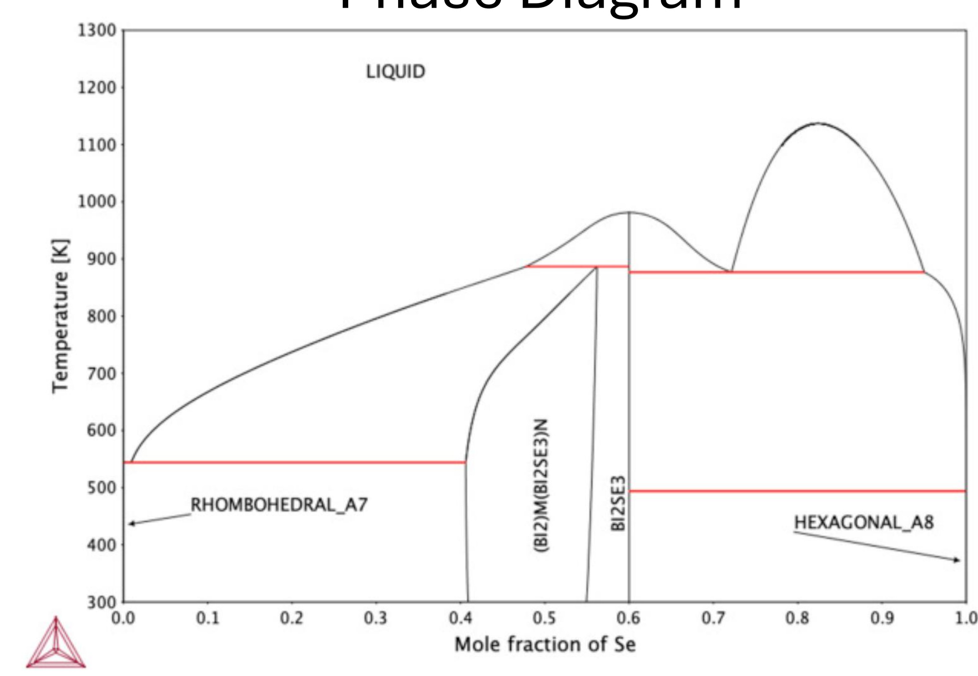
Sample Preparation: Bismuth (Bi) and Selenium (Se) were measured using a scale to match the stoichiometry of Bi_2Se_3. These elements were sealed inside an evacuated quartz ampule and placed in a furnace for melting and mixing. Once cooled, the ampoule was broken, and the material was ground into powder using a mortar and pestle for X-ray diffraction (XRD) analysis. The XRD results showed that the sample consisted of 86.9% Bi_2Se_3 and 13.1% of BiSe secondary phase, confirming that the composition was close to the desired one. The prepared material was then resealed in an ampoule and placed into the optical floating zone furnace.

Furnace Power Calibration: There is no established power-to-temperature relationship for this furnace, so it needed to be determined experimentally. Since Bi_2Se_3 melts at approximately 710°C, the furnace was initially set to 10% power. Power was then increased in 2% increments with each run to identify the power needed for melting. The material was observed to begin melting at 34% power, which established the baseline for future crystal growth trials.

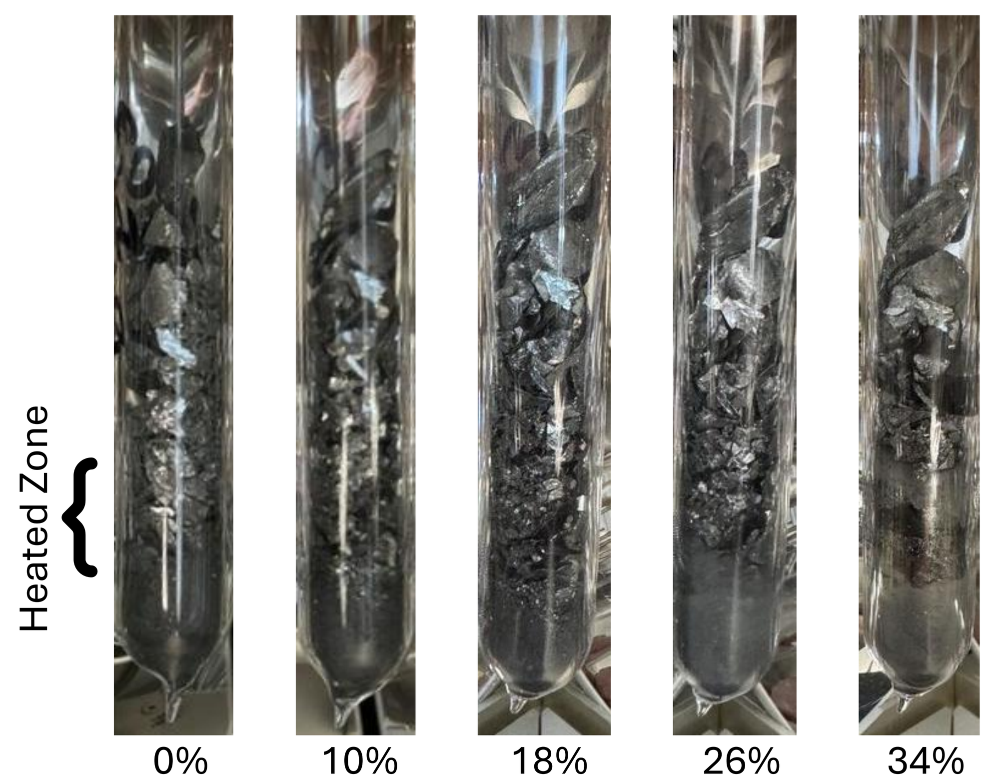
XRD Graph



Phase Diagram



Results & Discussion



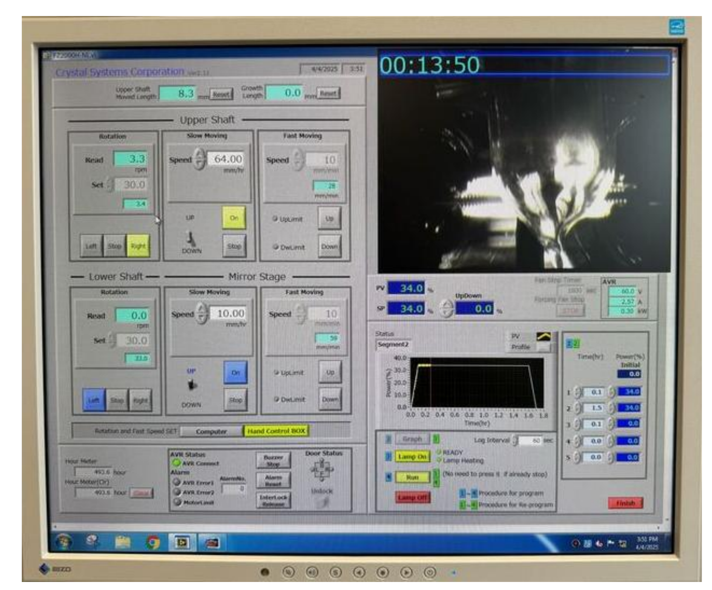
Close up on melting point (34%)

The images above show changes in the Bi_2Se_3 sample as furnace power increases. No clear visual changes are observed below 26% power. At 26% power, slight cloudiness begins to form, indicating that a reaction has occurred within the ampoule. At 34% power, a visible gap appears in the material, caused by molten Bi_2Se_3 flowing downward in the ampoule. Based on these observations, it can be concluded that 34% power corresponds to the melting point of the Bi_2Se_3 sample, which is approximately 710 °C.

Future Work

With the power required to melt Bi_2Se_3 established, the next step is to grow a single crystal from the sample. This will involve optimizing parameters such as upper and lower shaft movement, power ramp rate, rotation speed, and initial ampoule alignment.

Several other materials of interest to NASA—such as $CoSb_3$ and Bi_2Te_3—could also be synthesized using this method. These thermoelectric compounds are useful for space-based power systems, and producing high-quality single crystals may help improve their efficiency and reliability.



Optical Floating Zone Furnace Interface

References

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