

**Background and Proposed Research:** Over the last half a century, NASA has launched multiple deep space probes to discover the outer solar system and beyond. When low sunlight levels and dust aggregation makes photovoltaic energy sources undesirable, radioisotope thermoelectric generators (RTGs) become the key enabling technology. RTGs make use of thermoelectric (TE) materials to convert a temperature gradient (induced by a radioactive core and cold exterior) into a continuous power source. As a solid-state technology, RTGs have proven to be reliable for long periods of time; 46 years in the case of the Voyager missions [1].

NASA currently relies on thermoelectric materials such as SiGe and PbTe-TAGS in RTGs [2], but performance limits remain. Both are polycrystalline, as this structure provides mechanical stability and ease of fabrication, though grain boundaries reduce carrier mobility and thermal transport efficiency. A single crystal thermoelectric material would offer higher intrinsic electrical conductivity, reduced defect scattering, and more predictable anisotropic behavior, potentially improving the efficiency and longevity of future RTG systems.

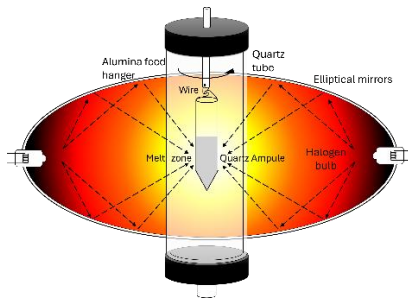


Figure 1: Optical Zone Furnace Interior

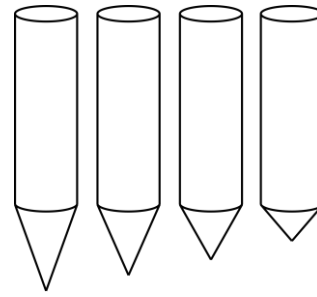


Figure 2: Ampule Shape Examples

The proposed research focuses on developing a controlled method for single crystal growth using the optical traveling zone method. Currently, only one other study has applied this approach to grow thermoelectric single crystal materials [3]. This method combines the precise temperature control of optical zone growth with the high-purity, vapor-sealed environment of an ampule, enabling systematic investigation of how parameters such as ampule geometry, translation rate, and temperature gradient influence crystal formation and quality.  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  are employed as model materials for this study because they are well-characterized, commercially utilized thermoelectrics whose sensitivity to growth conditions makes them ideal for exploring fundamental growth behavior.

Following synthesis, crystals will be characterized using X-ray diffraction (XRD) to assess structural quality, laser flash analysis (LFA) to measure thermal transport, and resonant ultrasound spectroscopy (RUS) to determine elastic properties and defect density. Correlating these results will establish how growth parameters affect microstructure and physical properties, providing insights applicable to a wide range of functional materials, including those used in NASA's thermoelectric power systems.

**Specific Aims:** The goal of this project is to investigate how growth parameters in an optical zone furnace influence crystal quality and physical properties.  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  are used as model

systems to study the mechanisms of translational crystal growth, with the broader aim of improving control and understanding of single-crystal synthesis methods relevant to thermoelectric materials used in NASA power systems.

- **Aim 1:** Develop and optimize single crystal growth procedures using an optical traveling zone method by systematically varying parameters
- **Aim 2:** Characterize the resulting crystals using X-ray diffraction (XRD), laser flash analysis (LFA), and resonant ultrasound spectroscopy (RUS).
- **Aim 3:** Correlate growth conditions with structural, thermal, and mechanical results to identify how specific parameters influence crystal quality.

### **Research Design and Methodology:**

**Synthesis:** All work will be conducted in Dr. Zevalkink's laboratory at Michigan State University. High-purity bismuth, selenium, and tellurium will be weighed in stoichiometric ratios, sealed under vacuum in cleaned quartz ampules, melted for homogenization, and slowly cooled to form polycrystalline precursors for zone melting.

**Single Crystal Growth (Aim 1):** Single crystals will be grown using the Crystal Systems Optical Floating Zone Furnace adapted for optical traveling zone (OTZ) growth. Source material sealed in quartz ampules will preserve volatile chalcogens and maintain a vapor-controlled, high-purity environment. The OTZ method provides precise, contact-free heating with steep thermal gradients for stable zone movement. Growth parameters (ampule geometry, translation and rotation rate, and temperature gradient) will be systematically varied to study their effect on zone stability and crystal quality.

**Characterizing Single Crystals (Aim 2):** Grown crystals will be characterized using X-ray diffraction (XRD) to assess lattice parameters, orientation, and phase purity; Laser Flash Analysis (LFA) to measure thermal diffusivity and conductivity [4]; and Resonant Ultrasound Spectroscopy (RUS) to determine elastic moduli and internal damping [5]. Together, these measurements will reveal how growth parameters influence crystallinity, thermal transport, and mechanical integrity.

**Analyzing Growth Parameters (Aim 3):** Experimental results will be correlated with growth conditions to identify trends linking synthesis parameters with structural, thermal, and mechanical behavior, determining the conditions that yield the most uniform and defect-free crystals.

**Relation to NASA's Strategic Interests:** This research supports NASA's strategic goals to expand human knowledge and enable long-duration exploration missions through the development of advanced materials and energy technologies. By improving understanding of single-crystal growth mechanisms in thermoelectric compounds, this work contributes to the foundation needed for higher-efficiency and longer-lasting radioisotope thermoelectric generators (RTGs), which power spacecraft in environments where solar energy is unavailable. The experimental approach also advances fundamental materials-processing knowledge relevant to in-space manufacturing and

defect control, aligning with NASA’s emphasis on sustainable, high-performance materials for space exploration (Strategic Goals 1, 2, and 4) [6].

**Student Responsibilities and Expected Outcomes:** I have worked in the Zevalkink Lab since February 2025, gaining experience in  $\text{Bi}_2\text{Se}_3$  single crystal growth using the optical traveling zone method, as well as in solid-state synthesis and x-ray diffraction analysis. In this project, I will perform ampule-based crystal growth of  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$ , systematically vary growth parameters, and conduct structural and thermal characterization. I will analyze how growth conditions affect crystal properties, with guidance from Dr. Zevalkink and a senior Ph.D. student, while learning to perform and interpret LFA and RUS measurements. The expected outcomes include optimized growth procedures, a dataset linking parameters to crystal quality, and a presentation of preliminary results at the 2026 MSGC Fall Conference.

**Impact Statement:** Establishing a reliable and well-documented method for growing single-crystal thermoelectric materials such as  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  will provide a foundation for producing high-quality crystals of other compounds relevant to NASA’s power systems. A clearer understanding of how growth parameters affect thermal and mechanical properties will guide the development of next-generation thermoelectrics optimized for radioisotope thermoelectric generators (RTGs) and other long-duration spacecraft power sources. This work will also contribute to the broader scientific effort to create efficient, defect-controlled materials for sustainable energy conversion technologies.

**Timeline:** The projected research timeline is shown in the Gantt chart below. The project will begin in August 2025 with material preparation and experimental setup, followed by single crystal growth trials using the optical traveling zone furnace through November. Characterization of grown samples using XRD, LFA, and RUS will occur concurrently with growth to guide parameter optimization and allow for material reusability. Data analysis and report preparation will take place in November and December, culminating in a final written report and presentation.

Table 1: Gantt chart indicating the general timeline of tasks

	August					September				October					November				December							
	1	8	15	22	29	5	12	19	26	3	10	17	24	31	7	14	21	28	5	12	19	26				
Material Synthesis / Setup																										
Crystal Growth – Ampule Geometry Variants (Aim 1)																										
Crystal Growth – Translation Rate Variants (Aim 1)																										
Characterization (Aim 2)																										
Analysis & Report (Aim 3)																										

**Future Plans:** Working in Dr. Zevalkink’s lab since February 2025 has inspired me to pursue a deeper understanding of materials research, leading me to add a Materials Science and Engineering minor to my Mechanical Engineering degree. This project has strengthened my interest in the relationship between material structure and performance, particularly in energy applications. After completing my undergraduate degree, I plan to continue to a master’s program in Mechanical and Materials Science Engineering, where I can build on this research experience and contribute to the development of advanced functional materials.

**References Cited:**

- [1] “Voyager – Planetary Voyage,” *NASA Jet Propulsion Laboratory*, <https://voyager.jpl.nasa.gov/mission/science/planetary-voyage/>.
- [2] J. P. Fleurial, “Thermoelectric power conversion materials for space and terrestrial applications,” *NASA Technical Reports Server (NTRS)*, NASA/CR–2016–001769, <https://ntrs.nasa.gov/api/citations/20160001769/downloads/20160001769.pdf>.
- [3] M. Stordeur and W. Streicher, “Preparation and properties of Bi<sub>2</sub>Te<sub>3</sub> single crystals,” *Crystal Growth & Design*, vol. 9, no. 12, pp. 4440–4444, 2009, doi: 10.1021/cg900675e.
- [4] R. Sundar and C. Sudha, “Thermal transport and thermal diffusivity by laser flash technique: a review,” *Int. J. Thermophys.*, vol. 46, article no. 13, 2025, doi:10.1007/s10765-024-03479-0.
- [5] F. F. Balakirev, S. M. Ennaceur, R. J. Migliori, B. Maiorov, and A. Migliori, “Resonant ultrasound spectroscopy: The essential toolbox,” *Rev. Sci. Instrum.*, vol. 90, no. 12, p. 121401, 2019, doi:10.1063/1.5123165.
- [6] *NASA Strategic Plan 2022–2026*, National Aeronautics and Space Administration, Washington, D.C., 2022. Available: [https://www.nasa.gov/sites/default/files/atoms/files/nasa\\_2022\\_strategic\\_plan.pdf](https://www.nasa.gov/sites/default/files/atoms/files/nasa_2022_strategic_plan.pdf).