

THESIS

ADVANCED SUBLIMATION SOURCE

FOR CDTE PHOTOVOLTAICS

Submitted by

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ABSTRACT

ADVANCED SUBLIMATION SOURCE FOR CDTE PHOTOVOLTAICS

This thesis presents the design, modeling, and validation of an advanced sublimation source for cadmium telluride (CdTe) thin-film photovoltaic (CPV) manufacturing, to improve thermal uniformity, system maintainability, and compatibility with Colorado State University's Advanced Research Deposition System (ARDS). Traditional heater configurations in close-space sublimation (CSS) processes have relied on nichrome (NiCr) heater coils cemented to graphite. These are prone to failure from thermal voids in the ceramic cement, dielectric breakdown, and complex maintenance and procedures. After several iterations a new source design incorporating split-sheath cartridge heaters used in the industry was developed and evaluated to address these limitations.

Steady-state thermal simulations in finite element software, ANSYS Mechanical, were performed to assess the impact of heater layout, graphite source geometry, and power distribution on temperature uniformity in the CdTe vapor region. G330 graphite with a thermal conductivity of $107 \text{ W/m}\cdot\text{K}$ was modeled. The effect of shielding and power output of the heater was included in the simulations. The simulations showed thermally uniform sources all within acceptable limits to meet a $\pm 10\%$ deposition uniformity.

The simulations showed that a 1.25" thick bottom plate produced the most uniform isothermal distribution, with less than $5 \text{ }^\circ\text{C}$ temperature variation across the region. These results were validated through experimental deposition and profilometry, which revealed $\pm 2.9\%$ thickness variation in CdTe films under typical processing conditions. In contrast to prior CSU

designs, such as the cemented NiCr configuration, the split-sheath system demonstrated improved thermal stability, maintainability, and resistance to arcing under vacuum.

This work confirms that split-sheath heaters and optimized source geometry offer a scalable and resilient solution for precision sublimation in next-generation CdTe PV manufacturing platforms.

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TABLE OF CONTENTS

ABSTRACT.....	ii
ACKNOWLEDGEMENTS.....	iv
LIST OF FIGURES	vii
1. Introduction.....	1
2. Background.....	3
3. Research Objectives.....	7
4. System Design and Methodology	9
4.1 Integration Constraints and Heater Selection.....	9
4.2 Graphite Source Geometry	12
4.3 Finite Element Modeling Approach	13
4.4 Preliminary Heater Expansion Testing.....	15
4.5 Experimental Methodology	17
5. Results and Discussion	18
5.1 Thermal Simulation Results	18
5.1.1 Temperature Distribution and Uniformity	18
5.1.2 Heater Failure Scenario	21
5.2 Comparison with Historical CSU Modeling (Walters, 2011)	22
5.3 Experimental Validation.....	23
5.3.1 CdTe Film Thickness Results	23
5.3.2 Heater Performance and Reliability	25
6. Conclusion and Future Work	27

6.1	Summary of Key Results	28
6.2	Future Work.....	28
	Publication	30
	REFERENCES	31

LIST OF FIGURES

Figure 1: Heater Failure due to air bubble	6
Figure 2: Assembled split sheath-heater configuration and graphite source.	9
Figure 3: Graphite Source with Cemented Heaters	11
Figure 4: Proposed Source Design.....	12
Figure 5: Mirror-like surface finish	14
Figure 6: Split-sheath expansion.....	15
Figure 7: Preliminary test, single bore.....	16
Figure 8: 1000W preliminary test.....	16
Figure 9: Source with 1.25" bottom thickness.....	19
Figure 10: Source with 0.75" bottom thickness.....	20
Figure 11: Source with 0.375" bottom thickness.....	21
Figure 12: Source with double heater failure.....	22
Figure 13: Thickness uniformity.....	23
Figure 14: Research Test Chamber setup	25
Figure 15: Bus shield post-test inspection	26

1. Introduction

The world is experiencing a new energy reality, with increased concerns over climate change, fossil fuel use, and a quest for sustainable sources. Solar photovoltaic technology has quickly become the foundation of the world's energy shift with its scalability, declining price, and unparalleled applicability on all scales of applications. Based on the 2025 Global Market Outlook for Solar Power, 2024 was the turning point year for the market: solar installations worldwide achieved a record-breaking 33% year-on-year growth of nearly 600 GW, driving the cumulative installed base past two terawatts (TW) for the first time. It had taken around seven decades for the first terawatt, but just two years to double it. That year, solar comprised 81% of all new renewables capacity additions and now provides around 7% of the world's power, almost twice its share three years earlier [5].

This explosive growth is fueled by accelerating progress in materials, mass production, and energy efficiency, along with historically low system cost due to global manufacturing overcapacity. Though its share of the energy mix remains modest compared with fossil fuels, solar PV is now leading all other power generation technologies in new capacity additions and electricity production. In 2024, it will grow three times as fast as wind and ahead of coal, gas, hydro, and nuclear in almost all major world regions.

Among the several photovoltaic technology options currently on the market, cadmium telluride (CdTe)-based thin-film solar cells have become one of the most promising for industrial-scale use. CdTe boasts numerous material and economic benefits compared with conventional crystalline silicon-based cells. It has a high optical absorption coefficient, allowing considerably thinner absorber layers to be used while lowering material expenses and processing time. In addition, CdTe modules have a relatively short energy payback period and are well adapted to for in-line vacuum manufacturing processes. This technology's business prospects are

demonstrated by the success of organizations like First Solar, reporting efficiencies in modules over 21 percent and production cycle time of less than five hours.

In addition to the economic and manufacturing advantages of CdTe thin-film photovoltaics, their environmental footprint is among the lowest in the PV sector. Life-cycle analysis comparing multiple PV technologies has shown that CdTe systems emit significantly less CO₂-equivalent per kilowatt-hour generated than crystalline silicon or fossil-fuel-based electricity generation. Alsema, de Wild-Scholten, and Fthenakis demonstrated that CdTe modules can achieve emissions below 20 g CO₂-eq/kWh and energy payback times of less than one year, depending on installation location and system design [6]. These attributes make CdTe technology cost-effective and environmentally preferable, especially when deployed at scale.

Despite these strengths, CdTe production remains subject to serious thermal process control issues, with significant difficulties associated with the absorber layer deposition sublimation stage. The widely employed close-space sublimation (CSS) method depends on a uniform and even heat distribution to facilitate stable deposition of the CdTe absorber layer. CFD and finite-element thermal modeling have become critical tools for predicting vapor transport and heat distributions in such systems, allowing for optimization of both source geometry and strategies for heating before experimental implementation is attempted [3]. Fluctuations in heater function or temperature gradients on the face of the heat source can result in inhomogeneous material transport, non-uniform grain growth, and, in turn, reduced device performance. Localized thermal inhomogeneity during CdTe sublimation has been shown by recent research to contribute to grain structure and electrical properties directly, further emphasizing the necessity for tight control of heat distribution in the vapor source region [1].

The drivers for this thesis lies in the desire to enhance the reliability, efficiency, and maintainability of the heater subsystems employed in Colorado State University's CSS reactors. Legacy systems employ cemented nichrome coils that have found widespread use in research-scale vacuum conditions despite documented deficiencies in uniformity, maintainability, and long-term reliability. Industry familiarity with split-sheath heaters that increase in diameter under thermal loading to produce substantial mechanical and thermal conformance indicates that the component may minimize installation complexity, improve thermal performance in vacuum conditions, and reduce power consumption [2]. Existing heater designs have depended on graphite crucible-based cartridge heaters cemented in position. Despite providing years of experimental research utility, such systems contribute considerably to thermal resistance, maintenance issues, and long-term reliability issues. This effort endeavors to resolve those deficiencies by creating, modeling, and testing an alternative heater design with eventual integration into the CSU's Advanced Research Deposition System (ARDS). The investigation examines a split-sheath heater design that promises improved thermal contact, enhanced uniformity, decreased power consumption, and easier replacement protocols.

2. Background

CSU's early breakthroughs in CdTe manufacturing were rooted in developing continuous, inline deposition systems capable of supporting high-throughput sublimation. Sampath, Barth, and Enzenroth detailed a system that utilized IR-lamp-heated graphite sources in a vacuum environment to sublime CdTe onto TCO-coated glass substrates [7]. This design became the basis for industrial-scale implementations by technology transfer partners and highlighted the importance of compact thermal sources with precise time-temperature control. However, their work also exposed the practical limitations of these early designs, including inconsistent film quality due to heater alignment, shielding degradation, and labor-intensive maintenance. These

observations laid the groundwork for future iterations, like the current split-sheath system described in this thesis.

The architecture of a CdTe solar cell consists of several functional layers deposited on a transparent conductive oxide-coated glass substrate. The device stack starts with a cadmium selenium telluride (CdSeTe) window layer, followed by the cadmium telluride absorber layer, the primary light-harvesting material. A metallic back contact completes the cell. Among those layers, the deposition of the CdTe absorber layer is of essential importance since it controls crystal structure, charge transport, and long-term stability of the solar cell. Thin-film uniformity, notably grain size and density, is directly related to temperature control during sublimation, as Shrivastava et al. have shown that non-uniform temperature fields during CSS growth can decrease open-circuit voltage and increase series resistance [1].

At CSU, the primary technique for depositing CdTe has been by close-space sublimation, in which the source and substrate are held in relatively proximity in vacuum, with the source being heated up past the sublimation point of CdTe and the substrate kept at a lower temperature to facilitate deposition. Proper deposition involves careful thermal control to prevent non-uniformities in the layer's thickness and crystal quality. Typically machined out of high-purity graphite, the source block has several vapor wells containing CdTe material. In the past, heat was transferred through embedded heaters installed with a ceramic cement to facilitate contact between the nichrome coils and graphite.

This cement-heater design, although initially successful in providing adequate power to the source, has shown several serious disadvantages over the years. Upon exposure to high vacuum temperatures, the ceramic cement outgases, creating virtual leaks that degrade the base pressure and potentially contaminate the thin-film deposition. Moreover, the inflexibility of the

encapsulation proves difficult to remove, frequently requiring destructive mechanical removal that may compromise the graphite body or cause misalignment upon replacements in subsequent heater installations. Thermal mismatches in expansion between the NiCr heater coil and cement can also cause stress concentrations, leading to premature failure.

Trapped air bubbles in the body of the cement create a serious problem. Under vacuum and thermal cycling, the bubbles are potential hot spots, allowing localized heating and failure. An illustration of such a failure in an earlier version of the cemented NiCr heater concept in CSU is presented in Figure 1. A visible rupture is evident, with discoloration and pitting in the surrounding region—characteristics of a breakdown event caused by a gas void. This type of degradation damages the heater and releases particulates into the chamber, compromising process reliability and driving increased maintenance needs. In addition to mechanical and contamination issues, the cement layer also creates inhomogeneous thermal conduction and emissivity variation along the heater interface, which has been demonstrated to generate temperature gradients along the graphite face. These gradients can directly cause non-typical CdTe film thickness and grain structure variation, ultimately affecting device performance and repeatability.



Figure 1: Heater Failure due to air bubble

Breakthroughs in thermal modeling in CSU, such as those by Walters (2011), emphasized the need for careful enclosure geometry, shielding, and heater contact arrangement in ensuring thermal uniformity. Other modeling outside of CSU, such as simulations of AP-MOCVD systems for CdTe, further indicates the capability of CFD and finite element analysis in modeling deposition uniformity and influencing reactor design [3]. Employing ANSYS Fluent, Walters created simplified, detailed thermal models of embedded NiCr heaters in graphite sources. These were compared with experimental measurements and showed that even slight design betterments in contact geometry and shielding would dramatically minimize thermal non-uniformity.

Concurrently, newer heater technology in split-sheath cartridge heaters became commercially accessible. The heaters grow radially when turned on, providing tighter contact with the bore wall and minimizing the necessary thermal filler material. They also do this with higher temperature ratings and increased durability. Manufacturers have seen that split-sheath heaters make it possible to obtain lower power operation and longer lifespan with easier removal and

replacement. While there are several benefits, no publication exists on applying split-sheath heaters to sublimation processes for CdTe thin-film PV. This thesis fills that gap by analyzing the application of split-sheath heaters in a sublimation source for the ARDS. By combining finite element analysis with experimental verification, the research comprehensively compares thermal performance, maintenance feasibility, and the effect of heater positioning and source block geometry on CdTe deposition uniformity.

One of the key advantages of split-sheath cartridge heaters is their ability to expand radially during operation, thereby improving thermal contact with the bore wall. Unlike cemented heaters, which often suffer from non-uniform conduction due to rigid encapsulation and contact gaps, split-sheath designs adapt to bore geometry and eliminate the need for thermal fillers. According to Dalton Electric, the manufacturer of the Watt-Flex split-sheath heaters used in this study, this design results in up to 40% more uniform heating compared to traditional round-sheath cartridges. This performance improvement is attributed to the heater's ability to center itself in the bore and eliminate conduction voids—an essential feature for ensuring uniform sublimation in CdTe processing environments.

3. Research Objectives

This thesis aims to design a heater configuration with increased thermal uniformity during CdTe sublimation. By utilizing a split-sheath design and removing cemented interfaces, the new design should minimize virtual leaks, ease maintenance, and improve long-term reliability in vacuum deposition conditions. This aligns with broader industry efforts in reducing the variability in CdTe module fabrication and production scale-up without compromising performance [4]. The project is expected to facilitate the integration of this heater design into the

Advanced Research Deposition System at CSU, allowing both enhanced experimental repeatability and closer approximation of industrial processing conditions.

To achieve this, the research pursues several related objectives. First, there is mechanical and thermal integration of an array of split-sheath heaters into a machined graphite block source. The geometry of the heater distribution and the source's dimensions—specifically the bottom plate's thickness—are changed to evaluate their impact on temperature uniformity in the vapor well region. Second, finite-element analysis in ANSYS Mechanical is carried out in steady-state conditions to analyze heat distribution for all the arrangements. The study includes radiation, conduction, and material emissivity in vacuum conditions.

Third, empirical verification of the simulated results is performed. A hardware heater assembly is created and integrated into a vacuum system, where the surface temperatures are measured and deposition experiments are carried out. CdTe films are deposited with controlled conditions, and their thickness is determined in several areas for determining spatial uniformity. The measurements are applied for correlating process outcomes with heater configuration.

Last but not least, the project gauges the long-term reliability and maintainability of the designed heater. Installation ease, vacuum arcing danger, heater replaceability without impairing the graphite crucible, power efficiency, and temperature ramp-up are weighed against one another. By this synergy of simulation, experiment, and system-level analysis, the project hopes to offer a scalable real-world solution for commercial use and extended PV research at CSU.

Figure 2 shows the finalized heater system with a Dalton Electric split-sheath heater inserted into a precision bore in the G330 graphite source. The terminals are housed in an alumina silicate bus shield, mechanically secured with ceramic hardware. This configuration was

designed for integration into the ARDS platform and evaluated via modeling and experimental validation.

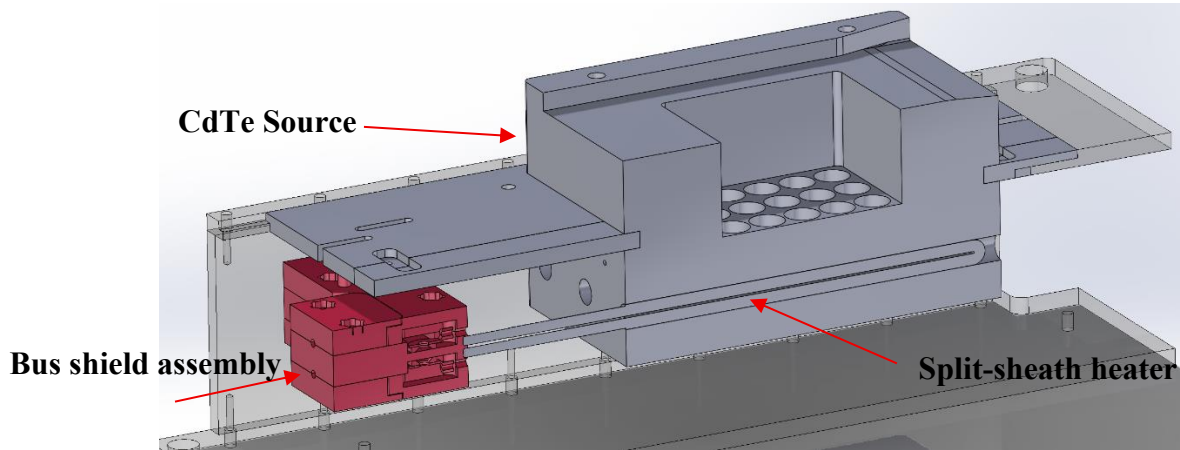


Figure 2: Assembled split sheath-heater configuration and graphite source.

4. System Design and Methodology

The heater configuration described in this thesis was developed for eventual deployment in the Advanced Research Deposition System (ARDS) at Colorado State University. This modular, load-lock vacuum deposition platform is explicitly designed for thin-film photovoltaic research. The ARDS allows researchers to experiment with various process parameters while maintaining a clean, repeatable environment across multiple deposition stations. Given the precision required in close-space sublimation (CSS) processes, the heater source intended for integration into the ARDS had to satisfy thermal performance requirements and strict criteria for reliability, maintainability, and scalability.

4.1 Integration Constraints and Heater Selection

After exploring many options, the heater chosen for this study is a commercially available split-sheath heater manufactured by Dalton Electric. Unlike traditional fixed-diameter cartridge

heaters, split-sheath heaters are engineered to expand radially when energized. This expansion improves the thermal interface between the heater and the bore of the graphite source block, thereby reducing the thermal contact resistance without the need for intermediary filler materials or cement.

Split-sheath cartridge heaters were selected for their ability to expand upon energization, creating intimate thermal contact with the surrounding bore surface without the need for thermal paste or cement. These heaters have a demonstrated history of performance in vacuum environments, as confirmed by prior industrial users and supported by the manufacturer. A previous customer of Dalton Electric noted that the heaters function well in vacuum systems as long as the surrounding material has sufficiently high emissivity. Graphite, particularly G330 used in this system, exhibits an emissivity typically ranging from 0.7 to 0.85 at elevated temperatures, depending on surface finish and oxidation. This property enables efficient radiative heat transfer within the chamber and aligns with the thermal coupling strategy assumed in the simulation and validated experimentally. The heater's compatibility with vacuum, combined with graphite's radiative properties, made this configuration ideal for integration into CSU's ARDS.

In legacy systems used at CSU, nichrome coils were installed into machined channels with a high-temperature ceramic cement, as seen in Figure 3. While effective, this approach introduced long-term reliability issues such as outgassing, arcing from exposed leads, premature failures due to air pockets, and difficult heater replacement. These challenges necessitate exploring alternative heater designs that can maintain high thermal contact while simplifying installation and removal. Split-sheath heaters expand radially during operation and offer improved mechanical fit and heat transfer performance without relying on cement or filler

materials. This makes them particularly attractive for vacuum applications where contaminant outgassing and terminal stress are concerns [2].

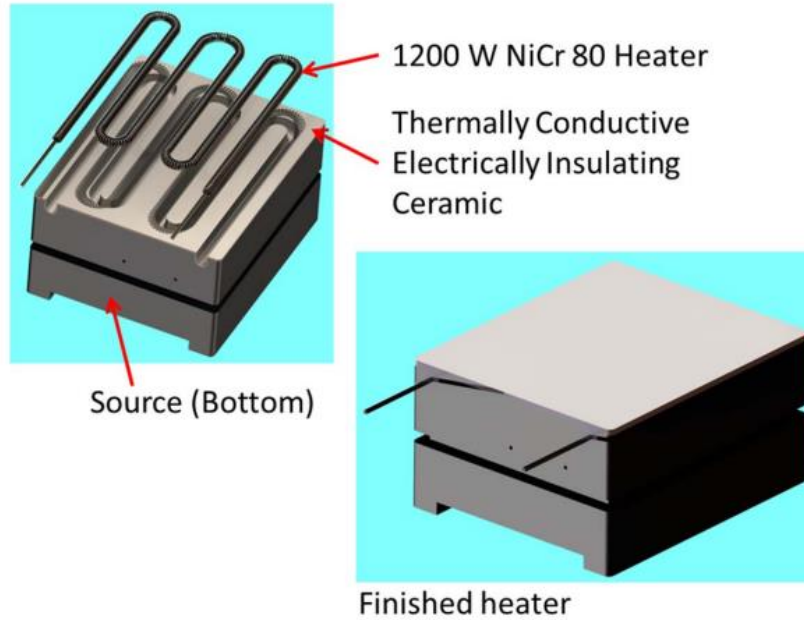


Figure 3: Graphite Source with Cemented Heaters

Each heater in the proposed configuration in Figure 4 is rated for 250 watts of power at 110 volts AC and is designed to withstand sheath temperatures up to 1000°C. For this application, the heaters were inserted in reamed bores in the graphite source block and installed with a lateral alignment consistent with previous heater studies conducted by Walters (2011).

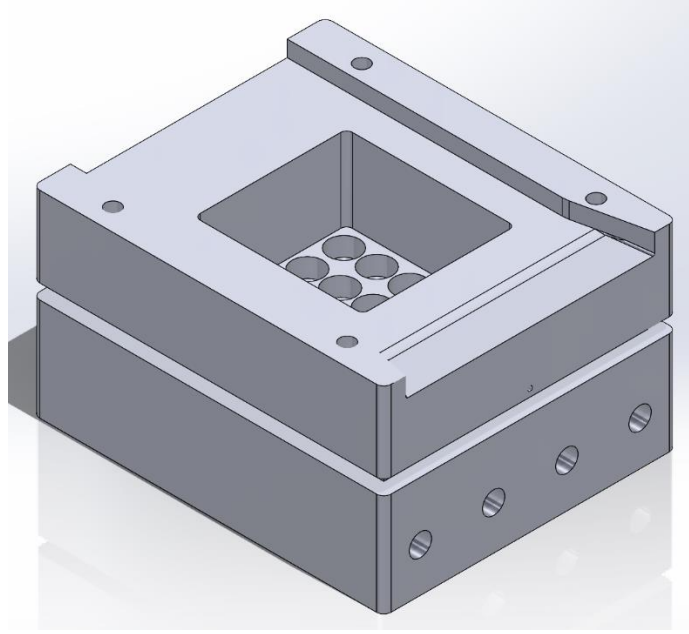


Figure 4: Proposed Source Design

4.2 Graphite Source Geometry

The heater array was inserted into a machined graphite block, which served as the primary CdTe vapor source. The design includes a flat upper surface featuring a grid of circular wells to contain cadmium telluride material prior to sublimation. These wells represent the “active” region of the source where uniform heat distribution is most critical. The source block was fabricated from high-density, high-purity graphite with an isotropic thermal conductivity of approximately $107 \text{ W/m}\cdot\text{K}$ at operating temperatures.

To investigate the influence of block geometry on temperature uniformity, three bottom plate thicknesses were modeled and tested: 0.375 inches, 0.75 inches, and 1.25 inches. The goal was to assess whether increased mass and thermal buffering in the thicker configurations could lead to reduced thermal gradients in the vapor zone. Each configuration preserved the same heater layout and vapor well spacing to maintain comparability.

4.3 Finite Element Modeling Approach

This research relies heavily on numerical modeling to evaluate thermal behavior in the graphite source block and guide physical system design. The strategic use of simulation aligns with broader recommendations from the National Science Foundation’s Blue Ribbon Panel on Simulation-Based Engineering Science (SBES). Their report emphasized that modeling and simulation “are now essential to engineering innovation,” enabling rapid iteration, cost reduction, and more sustainable design practices [8]. By applying steady-state thermal FEA to heater design and optimization, this study leverages SBES principles to bridge conceptual development and empirical validation.

To predict the thermal behavior of the proposed heater designs, a series of steady-state finite element analyses (FEA) were conducted using ANSYS Mechanical. These models were structured to capture the dominant heat transfer mechanisms in a vacuum environment—primarily conduction within the graphite and radiation from exposed surfaces. Convective effects were omitted, as the process operates under low-pressure argon environments (typically 30–34 millitorr), where free molecular flow dominates and convection is negligible.

The graphite block was modeled as a three-dimensional, isotropic solid. The heaters were defined as fixed-power thermal sources using values calibrated from the electrical power rating and estimated contact area. Solver settings and assumptions followed best practices outlined in the ANSYS Fluent Theory Guide [9]. Material properties for graphite were assigned based on manufacturer data, and emissivity values were set to 0.8 for internal surfaces and 0.3 for exposed surfaces, in alignment with the shielding and enclosure conditions used in previous CSU modeling work. [10]

In the simulation, thermal contact resistance between the split-sheath heaters and the inner bore walls of the graphite was neglected. This assumption was justified by the high-quality mirror-like surface finish as shown in Figure 5 achieved during reaming of the bores, which promotes intimate contact with the expanding heater sheath. Additionally, graphite's high thermal emissivity and conductivity contribute to rapid heat spreading from the heater surface, further minimizing the localized effects of any minor contact resistance.



Figure 5: Mirror-like surface finish

Symmetry conditions were applied to reduce the computational domain, and boundary conditions were defined to reflect the thermal isolation of the test chamber. All simulations were run to convergence using a residual tolerance of 1×10^{-6} for thermal energy balance.

The simulation matrix included four main cases:

- A 0.375" bottom thickness, fully energized heater array
- A 0.75" bottom thickness, fully energized
- A 0.75" bottom thickness, with 50% heater failure to simulate a worst-case scenario
- A 1.25" bottom thickness, fully energized

These models were analyzed for temperature gradients within the vapor well region, maximum surface temperatures, and spatial temperature deviation from the geometric center to the outer wells.

4.4 Preliminary Heater Expansion Testing

Before integrating the split-sheath heaters into the full sublimation source, a series of bench-scale tests were conducted to observe mechanical expansion behavior and assess contact pressure within the graphite bores. The operating principle of the split-sheath heater relies on differential thermal expansion. The heater's internal flat sheath segment reaches higher temperatures more rapidly than the outer circular sheath, inducing radial expansion. This ΔT -driven deformation seen in Figure 6 exerts a light outward pressure against the bore wall, improving thermal contact without the use of filler material.

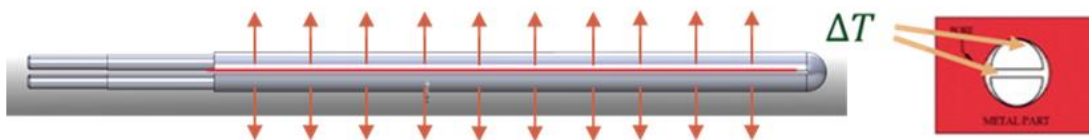


Figure 6: Split-sheath expansion

To verify this, a single-bore graphite block was machined to the same tolerance used in the full-size source. A split-sheath heater was inserted and energized under atmospheric conditions as shown in Figure 7. During and after heating, the heater could still be manually repositioned, indicating that while some expansion occurred, the applied contact pressure was minor. This finding is consistent with Dalton Electric's guidance that the heater is not intended to “lock” in place, but rather to improve thermal conduction through expansion and surface conformity.

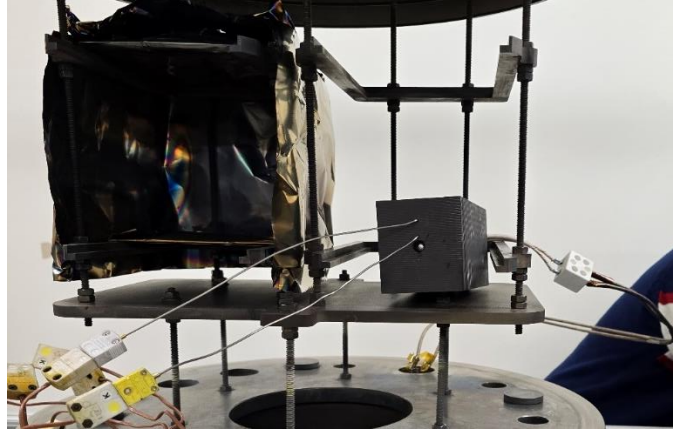


Figure 7: Preliminary test, single bore

A second test was performed on the complete four-bore assembly as shown in Figure 8. The source was fully energized at 1000W and reached a steady state temperature of 560 °C in 60 minutes. No deformation or galling of the graphite was observed. These results support the assumption used in simulation that contact resistance is negligible, particularly in combination with the bore's mirror-like surface finish and the high thermal emissivity of graphite.



Figure 8: 1000W preliminary test

4.5 Experimental Methodology

To validate the simulation results and assess practical implementation, a prototype source was fabricated and integrated into an experimental vacuum system with deposition capability. Surface temperatures were measured using embedded Type K thermocouples positioned in close proximity to the heater bores and within the vapor well region. The heaters were controlled using a Watlow EZ-ZONE PID controller.

CdTe films were deposited onto TEC12D soda-lime glass substrates coated with a conductive tin oxide layer. Deposition parameters were set to reflect realistic process conditions used in CSU's RTC chamber: a lower source temperature of 550°C, an upper source temperature of 500°C, and a process pressure of 30–34 millitorr using argon as the carrier gas.

Following deposition, film thickness was measured at five discrete locations—one at the center of the substrate and one at each corner—using a stylus profilometer. The data were analyzed to calculate average thickness, standard deviation, and percentage variation. The results were compared against the thermal maps generated in the FEA models, with a particular focus on the vapor well region where the temperature gradients were predicted to be most influential. Experimental evaluation also included tests of heater removal and reinstallation to assess maintainability. Visual inspections of the terminals and bus bar were conducted after extended use to assess any signs of arcing, carbon tracking, or contamination, particularly in the presence of cadmium and tellurium residue.

The combined modeling and experimental results provided a robust dataset to evaluate the proposed split-sheath heater configuration. The insights gathered informed not only the thermal design and integration strategy for ARDS, but also broader implications for future CdTe module manufacturing systems.

5. Results and Discussion

This chapter presents the results of the thermal modeling, experimental validation, and system performance testing conducted to evaluate the split-sheath heater configuration for CdTe sublimation. Simulation outputs are examined with respect to thermal gradients in the central vapor region, and these findings are compared to experimental deposition results and historical modeling data from Walters (2011) to assess consistency and improvement over prior designs.

5.1 Thermal Simulation Results

5.1.1 Temperature Distribution and Uniformity

Four steady-state thermal simulations were conducted in ANSYS Mechanical to evaluate the impact of graphite bottom plate thickness and heater configuration. The modeled configurations included bottom plate thicknesses of 0.375", 0.75", and 1.25", all using identical heater geometry and placement.

The graphite body was modeled using the properties of G330, a high-purity, fine-grain graphite known for its stability at high temperatures. Thermal conductivity was assigned as 107 W/m·K, consistent with manufacturer data for G330 in the 500–600 °C operating range. The model assumed isotropic conduction behavior, appropriate for the source's symmetrical and uniform geometry.

The simulations employed a symmetry condition, representing one-half of the full source. Experimental lab data determined that a total power input of 600 W is required to maintain the source temperature at 550 °C. For the half-model, this power was reduced to 300 W. Heat loads were distributed across four bore surfaces, with 75 W applied per surface, representing the effective thermal coupling between the split-sheath heaters and the internal graphite walls.

Although the actual system uses PID control for closed-loop feedback during operation, these simulations were performed under fixed-power, steady-state conditions to isolate passive

thermal behavior. The goal was to visualize isothermal contours in the vapor well region and evaluate lateral heat distribution under nominal conditions.

To account for the influence of radiative losses in a shielded vacuum environment, the surface emissivity was set to 0.3. This value reflects the partial enclosure and reflective baffle geometry surrounding the heater block, which reduces effective emissivity and radiative heat loss. This approach aligns with earlier work conducted at CSU for similar chamber environments. The 1.25" bottom thickness resulted in the most uniform temperature profile within the vapor well region, with a temperature difference (ΔT) of approximately 4.2°C between the hottest and coolest points. This configuration showed smoother lateral heat spreading and minimal hot spots near heater axes which can be seen in Figure 9.

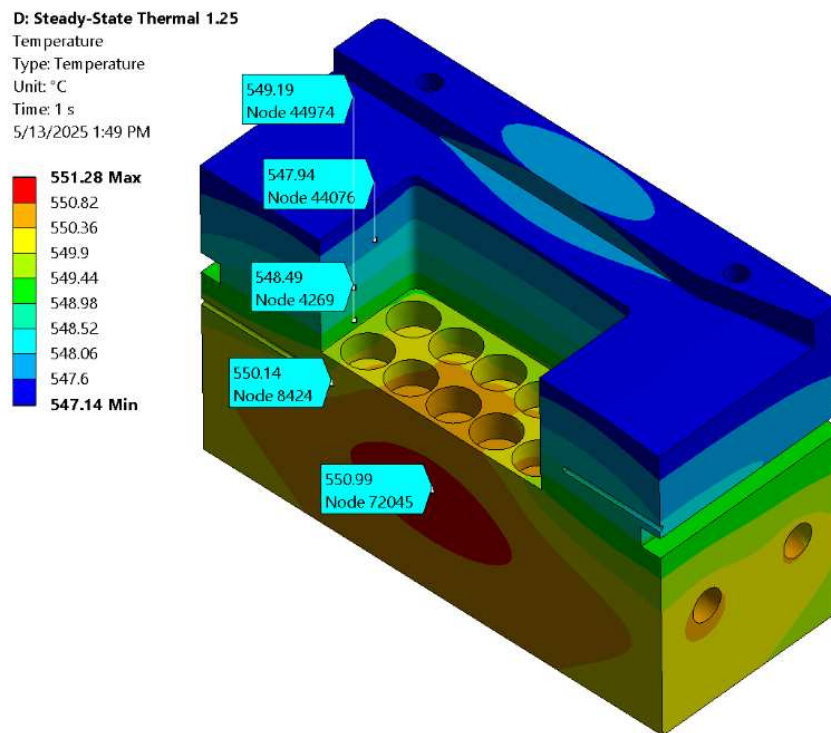


Figure 9: Source with 1.25" bottom thickness

The 0.75" bottom plate model displayed a ΔT of 4.6°C, slightly greater than the 1.25" case but still within acceptable uniformity limits. Thermal contours showed more pronounced local gradients near the heaters, particularly in regions adjacent to the outer wells which can be seen in Figure 10.

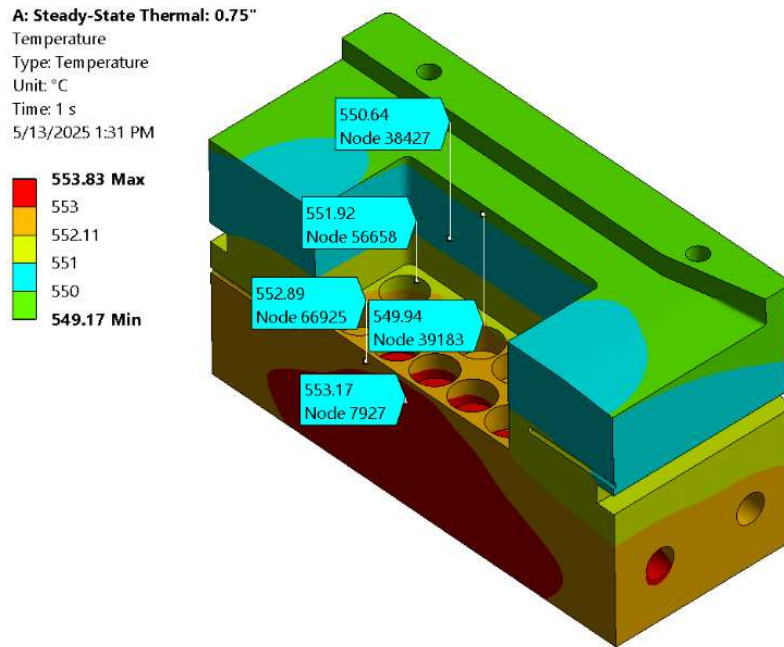


Figure 10: Source with 0.75" bottom thickness

The 0.375" configuration performed the worst, with a ΔT of 5.0°C across the well region which can be seen in Figure 11. The thinner plate exhibited sharp thermal gradients due to the lack of sufficient thermal mass to buffer spatial heat flux variation. This increased risk of local overheating, particularly at the heater interface, and would likely result in reduced film uniformity.

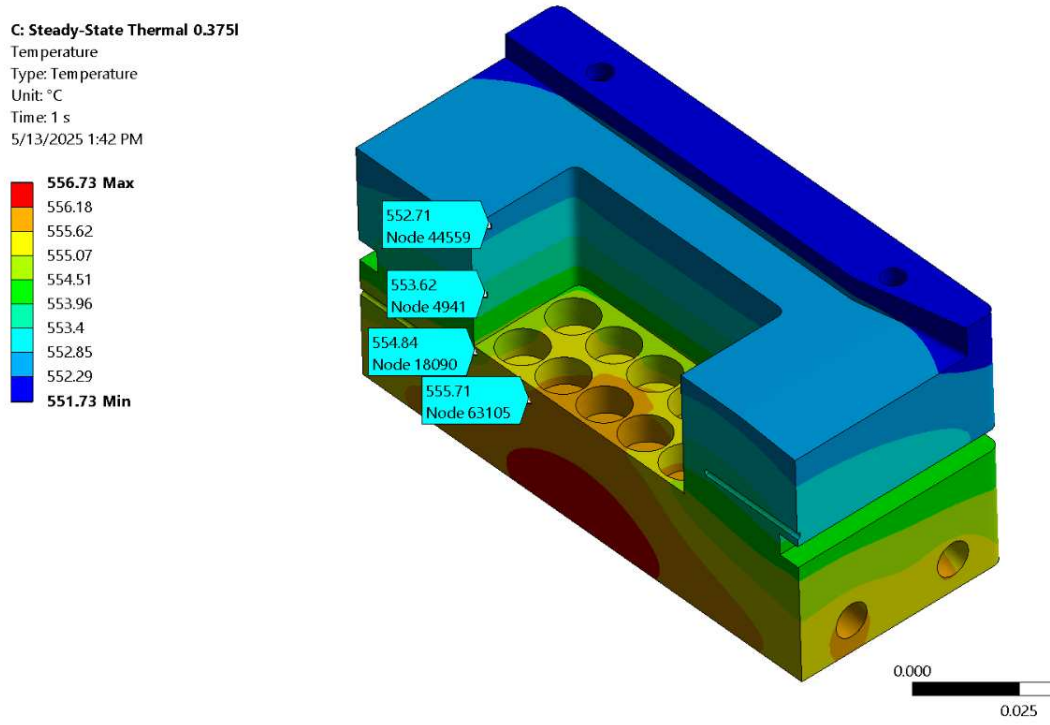


Figure 11: Source with 0.375" bottom thickness

5.1.2 Heater Failure Scenario

To evaluate the system's resilience under partial failure, a simulation was performed on the 0.75" plate with two heaters disabled, equivalent to 50% heater failure in the symmetric layout. The resulting ΔT increased dramatically to over 8°C, and temperature contours revealed strong asymmetry in heat distribution which can be seen in Figure 12.

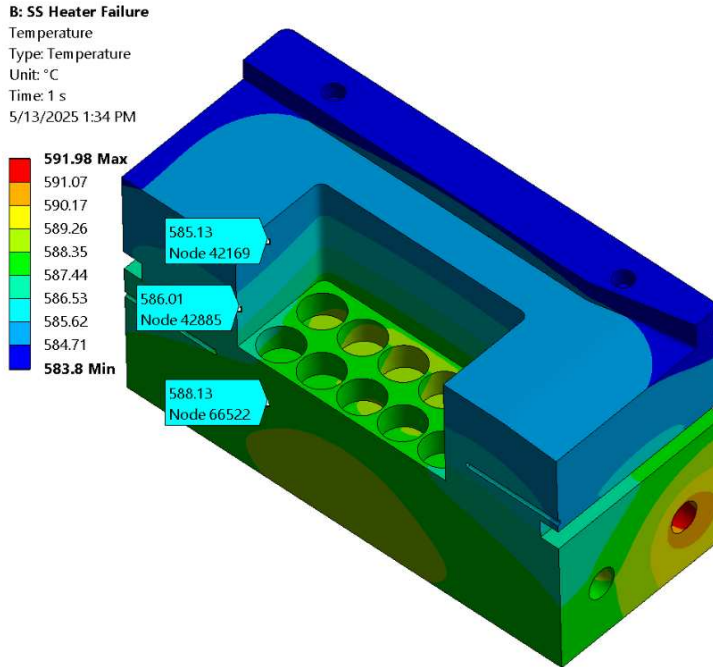


Figure 12: Source with double heater failure

This result reinforces the need for redundant heater coverage and real-time temperature monitoring. While the vapor region remained within the operating temperature range, the variation would likely introduce unacceptable spatial variability in CdTe deposition rate and morphology.

5.2 Comparison with Historical CSU Modeling (Walters, 2011)

In his 2011 thesis, Walters developed CFD-based thermal simulations for embedded NiCr heaters in graphite sources used in the earlier ARDS system. His models emphasized enclosure radiation, heater contact resistance, and shielding approximations.

Walters reported steady-state source temperatures of $\sim 555^{\circ}\text{C}$ for unshielded models and demonstrated temperature gradients of $7\text{--}12^{\circ}\text{C}$ across the heated graphite face under idealized conditions [2]. In comparison, the current split-sheath heater simulations exhibited improved thermal spreading, with temperature variations consistently under 5°C in the vapor well region.

The use of contact-expanding heaters also eliminates much of the contact uncertainty and variability noted in Walters' work.

5.3 Experimental Validation

5.3.1 CdTe Film Thickness Results

To validate the simulations, CdTe was deposited under controlled conditions using the 1.25" bottom plate configuration. Process conditions were set to 550°C for the lower source, 500°C for the upper source, and a chamber pressure of 30–34 mTorr with argon gas. There were no variations in temperature in the source, which validated the flat isotherms seen in the simulations.

Film thickness measurements were taken at five positions: the center and the four corners. The three corners and center measured 1.9, 1.9, 1.9, and 1.85 μm , respectively, while the fourth corner read 2.0 μm . This produced an average thickness of 1.91 μm and a standard deviation of 0.055 μm , or $\pm 2.9\%$ variation, as seen in Figure 13.



Figure 13: Thickness uniformity

These results confirm that the modeled thermal uniformity translates effectively into uniform material deposition. Film thickness deviations fall within industrially acceptable ranges and meet the internal $\pm 10\%$ criterion established earlier in the project.

To expand on the initial 2 μm deposition study, two additional films were produced with the improved split-sheath source, targeting nominal thicknesses of 100 nm and 300 nm. The 100 nm film had a measured standard deviation of 8 nm, while the 300 nm film showed a tighter distribution with a standard deviation of 14 nm. These results are consistent with the sub-10% uniformity goal and further demonstrate the effectiveness of the optimized heater design in maintaining consistent deposition even at sub-micron thicknesses.

For comparison, an additional 2 μm CdTe film was deposited using the original cemented-heater source design. This sample exhibited noticeably worse thickness variation, with a standard deviation of approximately 0.34 μm , corresponding to a 20% thickness deviation. This deviation exceeds the results observed from the split-sheath heater and supports the conclusion that the legacy design contributes to larger spatial thermal gradients and reduced film uniformity.

To further evaluate the vacuum compatibility of the split-sheath heater assembly and its alumina silicate bus shield, a test scenario was conducted in which the whole heater assembly was removed from the chamber. The system's ultimate base pressure was recorded both with and without the heater and shield installed under otherwise identical pump-down conditions. The results showed no measurable difference in base pressure (6 mtorr), confirming that the heater assembly and shielding materials do not contribute to virtual leaks, outgassing, or particulate contamination under vacuum. This supports the conclusion that the components are fully compatible with high-vacuum deposition environments and that their inclusion does not degrade chamber performance.

5.3.2 Heater Performance and Reliability

The split-sheath heaters operated continuously during an 80-hour thermal test in the Research Test Chamber without failure, as shown in Figure 14. Post-test inspection revealed no signs of carbon deposition, dielectric breakdown, or terminal arcing. The alumina silicate bus shield remained fully intact and free of particulate contamination, confirming the effectiveness of the dielectric protection and the shield's ability to isolate electrical connections under high-temperature, low-pressure conditions. Notably, two adjacent heater sources using the legacy cemented NiCr design experienced breaker trips during the same test period, while the split-sheath heater system continued to operate stably, maintaining a uniform temperature of 550 °C without thermal assistance from neighboring sources. This outcome underscores the robustness and reliability of the heater configuration described in this study. This result is shown in Figure 15.

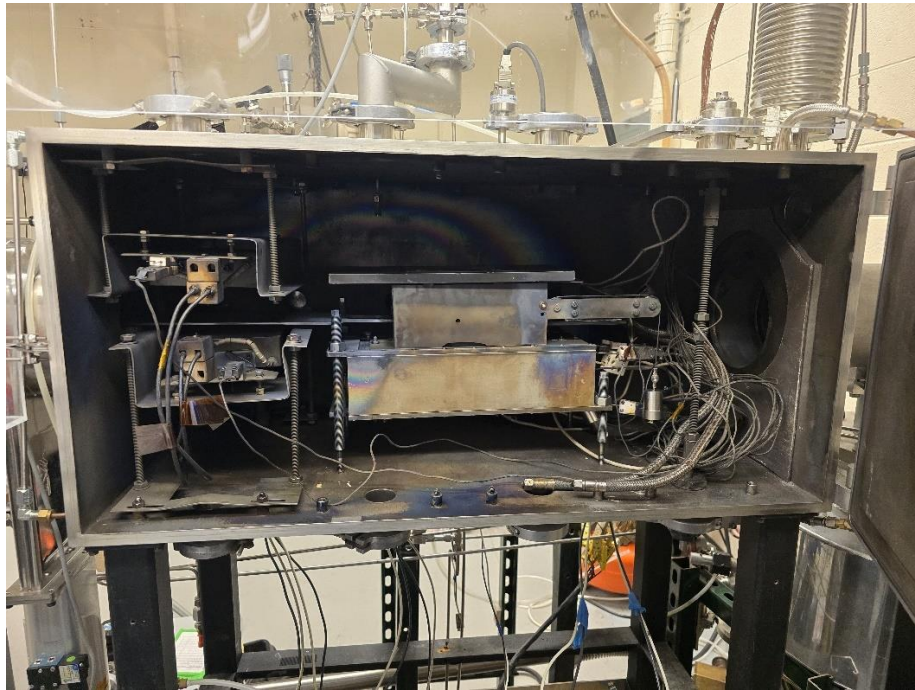


Figure 14: Research Test Chamber setup

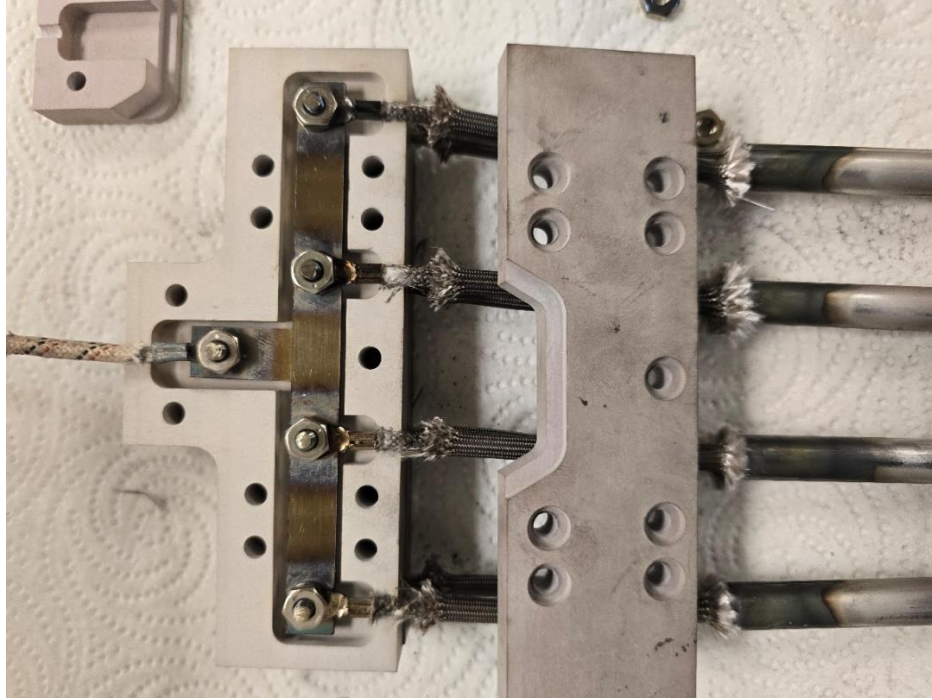


Figure 15: Bus shield post-test inspection

During extended vacuum testing, three thermocouples embedded in the graphite block indicated a steady-state operating temperature of 550 °C. However, we estimate a measurement uncertainty of ± 1 °C based on calibration tolerance and positional effects. Factors contributing to this include surface contact variation, lead routing through the vacuum flange, and possible radiative influence from nearby heaters. While all sensors consistently reported target temperatures, this uncertainty range should be considered when interpreting the comparison between modeled and measured thermal performance.

The heaters were also removed and reinstalled without damaging the graphite block or requiring re-machining. This validates the mechanical serviceability hypothesis and further supports the case for replacing cemented configurations with press-fit split-sheath designs.

6. Conclusion and Future Work

This thesis set out to investigate and validate a next-generation heater configuration for cadmium telluride (CdTe) sublimation, designed for integration into the Advanced Research Deposition System (ARDS) at Colorado State University. The study was structured around three primary hypotheses:

- H1: Split-sheath cartridge heaters would improve heat transfer efficiency and allow for easier installation and maintenance compared to traditional cemented heaters.
- H2: A properly designed alumina silicate terminal shield would prevent electrical arcing and contamination during high-temperature vacuum operation.
- H3: Optimizing the bottom plate thickness will maintain a one-hour ramp-up time to steady-state conditions while meeting H1 requirements.

The results of both simulation and experimental testing confirm that all three hypotheses were satisfied. Steady-state thermal simulations demonstrated that a 1.25" graphite bottom plate yielded the best thermal uniformity, with temperature gradients across the vapor well region maintained below 5 °C. In contrast to earlier heater models—such as Walters' cemented NiCr design—this split-sheath approach produced more uniform temperature fields, better alignment with experimental data, and reduced uncertainty related to heater installation.

Preliminary expansion testing confirmed that the split-sheath heaters exert a mild mechanical force on the bore walls when energized, sufficient to improve contact without damaging the graphite or restricting serviceability. Experimental deposition validated the simulation results: CdTe films exhibited a thickness variation of less than $\pm 3\%$, well within the industry's $\pm 10\%$ benchmark for uniformity. The heater system operated continuously during an 80-hour vacuum test, with no evidence of arcing or particulate contamination. In contrast, two adjacent sources built using earlier heater designs tripped breakers during the same operational period, while the

new source maintained stable temperature and uninterrupted performance. These findings underscore the robustness, scalability, and process compatibility of the heater design.

6.1 Summary of Key Results

- The 1.25" bottom plate provided the best thermal uniformity ($\Delta T \approx 4.2$ °C).
- The heater failure scenario emphasized the need for symmetry and redundant heater coverage.
- The split-sheath configuration outperformed CSU's prior NiCr heater designs in both modeling and validation.
- Experimental CdTe films deposited using the new source achieved <3% thickness variation.
- The heater system remained reliable and easy to maintain during extended operation in vacuum.
- The source maintained 550 °C setpoint autonomously, while other sources failed under identical test conditions.

Collectively, these results validate the suitability of the split-sheath heater design for ARDS integration and demonstrate its value as a robust, maintainable, and thermally consistent sublimation platform for CdTe photovoltaic research.

6.2 Future Work

While this study achieved its core objectives, several opportunities remain to improve system reliability, usability, and process control.

A key priority is the redesign of the electrical bus shield. The current shield—though effective—uses a five-piece construction that is sensitive to misalignment. The next-generation design will transition to a single-piece, monolithic ceramic shield with two precision-drilled cylindrical

bores to accommodate circular nickel bus bars. Set screws, accessed via external ports, will be used to secure the terminals, and ceramic end caps will protect the contact points from particle ingress. This revision is expected to simplify assembly, improve repeatability, and further reduce contamination risk.

Importantly, this shield redesign should not be limited to the lower source. The top heater and co-sublimation sources experience similar operational stresses in vacuum and should adopt a unified shield architecture. Standardizing this design across all ARDS heat sources would streamline maintenance procedures, reduce training overhead, and improve modularity. Beyond mechanical refinement, future studies should explore thermal zoning strategies and multi-zone PID control. While the current system uses uniform power delivery, segmented heating could enable greater control over lateral gradients, especially important for larger or multi-material deposition sources. Embedding additional thermocouples at key locations may support real-time thermal feedback and enable closed-loop correction of temperature asymmetries.

Finally, future modeling efforts should go beyond steady-state temperature analysis to incorporate species transport, sublimation rates, and film formation kinetics. Coupling these models with thin-film characterization data, such as grain size, optical absorption, and device efficiency, will allow researchers to connect thermal control directly to photovoltaic performance, closing the feedback loop between source design and module output. Through these refinements, the heater and source platform developed in this thesis can evolve into a comprehensive, high-performance solution for advanced CdTe, CdSeTe, and multi-layer thin-film research systems within CSU's ARDS framework and beyond.

Publication

M. Tapparo, A. Shah, and A. H. Munshi, "Investigation of Process Ambient on Performance and Characteristics of CdSeTe/CdTe Solar Cells," in *Proc. 2024 IEEE 52nd Photovoltaic Specialist Conference (PVSC)*, Seattle, WA, USA, Jun. 2024, pp. 1–4. [Online]. Available:

<https://ieeexplore.ieee.org/document/10749460/references#references>

REFERENCES

1. S. B. Shrivastava et al., “Effect of temperature non-uniformity during CdTe growth on film structure and electrical performance,” **Materials Today: Proceedings**, vol. 39, pp. 1195–1200, 2021.
2. Dalton Electric Heating Co., “Watt-Flex® Split Sheath Cartridge Heater Technical Specifications,” [Online]. Available: <https://www.daltonelectric.com>.
3. S. Khandekar and G. V. Soni, “CFD modelling of cadmium telluride (CdTe) thin film coating with inline AP-MOCVD,” **Journal of Mechanical Science and Technology**, vol. 27, no. 2, pp. 437–443, 2013.
4. A. Munshi et al., “Progress in CdTe solar cell performance through advances in materials, device structures, and processing,” *Solar Energy Materials and Solar Cells*, vol. 203, p. 110164, 2019. doi: 10.1016/j.solmat.2019.110164.
5. SolarPower Europe, *Global Market Outlook for Solar Power 2025–2029*, Brussels, Belgium, 2025. [Online]. Available: <https://www.solarpowereurope.org/insights/outlooks/global-market-outlook-for-solar-power-2025-2029/detail>
6. Alsema EA, de Wild-Scholten MJ, Fthenakis VM. Environmental impacts of PV electricity generation-a critical comparison of energy supply options. In: *21st European photovoltaic solar energy conference, Dresden, Germany*. Vol 3201.; 2006.
7. W.S. Sampath, K.L. Barth, R.A. Enzenroth. Advances in Continuous, inline processing of stable CdS/CdTe devices. Available at: <http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=01190624>. Accessed September 10, 2011.

8. W.S. Sampath, K.L. Barth, R.A. Enzenroth. Advances in Continuous, inline processing of stable CdS/CdTe devices. Available at:<http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=01190624>. Accessed September 10, 2011.
9. Anon. ANSYS Fluent Theory Guide. ANSYS Inc. Release 13.0, November 2010
10. K. E. Walters, *Computational Fluid Dynamics (CFD) Modeling for CdTe Solar Cell Manufacturing*, M.S. thesis, Dept. of Mechanical Engineering, Colorado State University, Fort Collins, CO, 2011.