High-efficiency Solar Thermophotovoltaic Systems Based on Spectrally

Selective Emitters

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Abstract

Recent advances in low-bandgap semiconductor materials for solar cell technology has generated renewed interest in the development of solar thermophotovoltaic (STPV) devices, given their potential for high-efficiency solar energy harvesting by utilizing the full solar spectrum. STPV systems aim to achieve efficiencies higher than the Shockley-Queisser (SQ) limit for photovoltaic conversion through the use of an intermediate element that absorbs the broadband sunlight and reemits the absorbed energy as narrow-band thermal radiation tuned to the characteristic spectral response of the solar cell. Spectrally selective absorbers and emitters can greatly enhance the STPV system efficiency by maximizing the absorption and suppressing the emission of sub-bandgap and excessive energy photons. STPV is a promising technology for building scalable, reliable, and maintenance-free high-energy-density electrical power generator systems. These features along with their versatility of utilizing numerous input sources of heat, such as concentrated solar energy, industrial waste heat, radioisotope heaters, combustible materials, etc., make thermophotovoltaic (TPV) systems very appealing for many terrestrial and space applications.

This dissertation study focused on the design, optimization, and fabrication of a fully operational high-efficiency planar STPV system comprising GaSb cells and spectrally selective emitters. Designing an efficient STPV system is a balancing act and requires a comprehensive understanding of all the loss mechanisms at various stages of the energy transport. A combination of thermodynamic modeling and transfer matrix method (TMM) simulation was used to formulate a detailed-balance analysis required for the design and optimization of high-performance selective surfaces that are essential components of efficient STPV systems. Significance of determining the optimal values of the emitter temperature, spectral cut-off wavelengths, absorber-to-emitter area ratio, and emitter bandwidth for global system optimization was discussed. The relevance of

photon recycling on both the absorbing and emitting sides for achieving high thermal extraction and overall system conversion efficiency was investigated.

Utilizing the knowledge gained from the simulation study, a high-efficiency planar STPV system was designed, fabricated and evaluated. A micro-textured selective absorber and a $Si_3N_4/W/Si_3N_4$ coated selective emitter were fabricated on a W substrate. The absorptivity of 0.92 was measured for the textured absorber for wavelengths below 1 µm. The selective emitter exhibited a high surface emissivity in spectral regimes matching the quantum efficiency of the GaSb solar cells. Photon recycling was incorporated to suppress the thermal emission loss within the system. The performance of the STPV system was evaluated using a 300 W continuous-wave laser as a simulated source for incident radiation. An output power density of 1.75 W/cm² and a system efficiency of 8.6% were recorded at the operating system temperature of 1670K. This experimental efficiency is higher than those of previously reported STPV systems. Various optical and thermal losses occurred at multiple stages of the energy conversion process were quantified.

This dissertation also studied the dependence of the surface spectral absorptivity upon temperature and quantified its impact on the performance of the selective emitter. The long-term thermal stability of the selective surfaces was also assessed. Combining the simulation and experimental results, essential guidelines to further improve the system efficiency were also provided.

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List of Symbols and Abbreviations

$B(\lambda, T)$	Planck's blackbody function
ε _{Eff}	Effective emissivity
Ein-band	In-band emissivity
η _e	Thermal extraction efficiency
ηρν	Photovoltaic conversion efficiency
η_{sel}	Spectral selectivity
' NSTPV	STPV system efficiency
λ	Wavelength
λ_{BG}	Bandgap wavelength
T	Absolute temperature
EQE	External quantum efficiency
eV	Electron volt
FF	Fill factor
GaSb	Gallium Antimonide
Ge	Germanium
HfO ₂	Hafnium oxide
InAs	Indium Arsende
InGaAsSb	Indium Gallium Arsenide Antimonide
IR	Infrared
Mo	Molybdenum
Pcond	Power loss due to conduction
P _{conv}	Power loss due to convection
Pin	Incident power
PECVD	Plasma-enhanced chemical vapor deposition
P _{ref}	Reflected power
P _{rad}	Thermally radiated power
PV	Photovoltaic
QTH	Quartz tungsten halogen
Si	Silicon
Si ₃ N ₄	Silicon Nitride
SQ	Shockley-Queisser
STPV	Solar thermophotovoltaic
Та	Tantalum
TMM	Transfer matrix method
TPV	Thermophotovoltaic
VF	View factor
W	Tungsten

Chapter 1: Introduction and Motivation

A single-junction solar cell is subject to the Shockley-Queisser (SQ) limit [1], which imposes a fundamental upper bound on its solar-to-electric energy conversion efficiency. According to this limit, the theoretical maximum efficiency for a single-junction cell under standard illumination (air mass of 1.5 and in the absence of concentration) is ~33% for an optimal bandgap of ~1.4 eV [2]. A major contribution to the SQ limit arises from two fundamental losses in the energy conversion process. One is due to the non-absorption of sub-bandgap photons that do not carry sufficient energy to create electron-hole pairs. Second, the excess energy of photons carrying greater energy than the bandgap (E_{BG}) of the solar cell is lost as heat during the thermalization process. STPV systems aim to achieve efficiencies higher than the SQ limit through spectral modification of the incoming solar radiation with the aid of an intermediate absorber/emitter element.

1.1 Solar thermophotovoltaic system overview

First proposed by Swanson [3] in 1979, a solar thermophotovoltaic (STPV) system offers a unique way of converting a concentrated solar energy into electricity. It utilizes an intermediate element that efficiently absorbs the incoming concentrated solar radiation and thermally re-radiates photons at tailored wavelengths matching with the spectral bandwidth of a target solar cell for optimal photovoltaic (PV) conversion. Spectrally selective absorbers and emitters can greatly enhance the STPV system efficiency by maximizing the absorption of the incident sunlight and suppressing the emission of both sub-bandgap and excessive energy ($E >> E_{BG}$) photons, thereby utilizing most of the solar spectrum for energy conversion [4].

The upper bound for STPV conversion efficiency can be derived by realizing an STPV system as an ideal solar-thermal engine [5], as shown in Figure 1.1a. At the most fundamental

level, the solar-thermal engine can be assumed to have two stages of energy conversion: solar-to-thermal conversion by the intermediate element and thermal-to-electric conversion by solar cells. The ultimate STPV efficiency (η_{STPV}) is the product of the efficiencies of the two intermediate stages.

$$\eta_{STPV} = \eta_{sol-th} \cdot \eta_{th-elec} \tag{1.1}$$



Figure 1.1: (a) Realization of an STPV system as an ideal solar-thermal engine. (b) Maximum η_{sol-th} , $\eta_{th-elec}$, and η_{STPV} as a function of the absorber/emitter temperature under fully concentrated sunlight and a blackbody absorber.

The maximal η_{sol-th} is achieved under maximal solar concentration incident on a blackbody

absorber, and is given by

$$\eta_{sol-th} = \frac{\sigma T_{Sun}^4 - \sigma T_A^4}{\sigma T_{Sun}^4} = 1 - \left(\frac{T_A}{T_{Sun}}\right)^4$$
(1.2)

where T_{Sun} is the surface temperature of the sun, T_A is the steady-state temperature of the blackbody absorber, and σ is Stefan–Boltzmann's constant. Similarly, the maximum value of η_{th-} elec is equal to the efficiency of a Carnot engine operating between two heat reservoirs and is given by

$$\eta_{th-elec} = 1 - \left(\frac{T_{ambient}}{T_A}\right) \tag{1.3}$$

where $T_{ambient}$ is the temperature of surrounding. The ultimate η_{STPV} is therefore given by Equation 1.4.

$$\eta_{STPV} = \left(1 - \frac{T_A^4}{T_{Sun}^4}\right) \left(1 - \frac{T_{ambient}}{T_A}\right)$$
(1.4)

Note that high T_A provides low η_{sol-th} but high $\eta_{th-elec}$ and vice-versa. The optimal value of T_A that maximizes η_{STPV} in Equation (4) is 2544 K, and the corresponding system efficiency is 85.4%, assuming T_{Sun} =6000 K and $T_{ambient}$ =300 K. Therefore, in theory, the STPV technology has the ultimate solar-to-electricity conversion efficiency limit that is close to the upper efficiency limit for an infinite number of stacked monochromatic solar cell junctions illuminated by a maximum solar concentration [6]. Maximum conversion efficiency as a function of STPV temperature is shown in Figure 1.1b. In addition, STPV systems are versatile and can utilize alternative sources of heat, such as radioisotope heaters, thermal storage systems, combustible materials, industrial waste heat, etc., as inputs when sunlight is unavailable.

1.2 Problem Statement

STPV is a promising technology for achieving high-efficiency solar energy harvesting to fulfill the future energy needs. Owing to the absence of any moving parts, STPV systems have potential to provide extremely reliable and maintenance-free electricity for a long period of time. They are highly scalable as well. These features along with the versatile fuel usage for heating the intermediate element make thermophotovoltaic (TPV) systems very appealing for terrestrial and space applications.

The derivation of the ultimate efficiency limit for an STPV device is simplified and based on several restrictive constraints that cannot be achieved in real systems. For instance, the maximum system efficiency is achieved at an impractical solar concentration of 46000X, with a narrow monochromatic emission (matching the bandgap of the cell) from the emitter and using solar cells with no optical losses and non-radiative recombination. The narrowband monochromatic emission requires extremely large (approaching infinity) emitter area to re-radiate the absorbed solar radiation, resulting in an impractical STPV system with nearly zero output power density [7]. A realistic STPV system is required to be more compact and produce adequately high output electrical power density from practically achievable input solar concentration. Therefore, the idea of monochromatic emitter needs to be abandoned and the thermal emission from the emitter is required to have a sufficient bandwidth to maximize the open circuit voltage and impedance matching in PV cells [4]. However, increasing the bandwidth far above the bandgap may result in increased thermalization loss. Similarly, the input side of a STPV system should exhibit high absorptance to solar input. Because a good absorber is a good emitter too, there are back radiation losses from the absorber side. Nonetheless, in a more practical STPV system, there are conversion losses due to cell efficiency, conduction heat losses from support systems, and cavity losses due to non-unity radiative view factor (VF) between the emitter and PV cells, and loss due to the emission of sub-bandgap photons. Designing a high efficiency STPV system is, therefore, a balancing act and requires a comprehensive understanding and optimization of all the loss mechanisms at various stages of energy transport.

This thesis aims to explore the integral components of a less idealized STPV system in great detail and provide a complete thermodynamic analysis that would provide the demonstration of high-efficiency STPV devices.

1.3 Objective

Despite the significant potential of STPV systems, very few experimental results have been reported so far. The primary objective of this dissertation is to design, optimize, and fabricate a high-efficiency planar STPV system utilizing a tungsten-based selective absorber/emitter structure. The spectral property of the absorbing surface is modified to achieve high absorbance at visible and near-infrared wavelengths. The surface emissivity of the emitter is tuned to match the quantum efficiency of GaSb solar cells. First, a complete thermodynamic simulation model is formulated to investigate energy transport processes among different components of the STPV system and quantify losses at the multiple stages during the energy conversion process. Desired optical properties of the selective absorbing and emitting surfaces are computed and optimized through numerical simulation using transfer matrix method (TMM). The simulated results are validated using experimental methods. Based on the knowledge acquired from the simulations, a complete STPV system is designed, fabricated, and tested. The fabrication process, experimental procedures, and results are discussed in detail. Combining the results from simulation and experiment, a necessary framework for further investigation and towards improving the overall system efficiency is provided. In addition, this dissertation investigates the temperature dependence of the spectral properties of the selective surfaces and its overall impact on the system performance. The thermal stability of the STPV system at high temperature is also evaluated.

Chapter 2: Fundamentals of STPV System

2.1 Fundamentals of Thermal Radiation

Thermal radiation is emitted by all objects with temperatures above the absolute zero (-273.15 °C) and is radiated in the form of electromagnetic waves. The amount of radiation energy emitted from a surface is determined by the material of the body and its surface temperature [8]. This means different bodies at the same temperature may emit different amounts of thermal radiation. For a given temperature, the maximum amount of radiation is emitted by an idealized body, called a blackbody, that is defined as a perfect emitter and absorber of radiation. The blackbody provides a reference against which the radiative properties of real surfaces are compared. The spectral emissive power, B(λ , *T*), radiated by a blackbody surface is provided by the Planck's equation given below.

$$B(\lambda, T) = \frac{C_1}{\lambda^5 [\exp(\frac{C_2}{\lambda T}) - 1]}$$
(2.1)

where $C_1=3.742 \times 10^8 \text{ W.}^\circ \mu \text{m}^4/\text{m}^2$, $C_2=1.439 \times 10^4 \mu \text{m}$. K, λ is the wavelength of radiation emitted, and T is the absolute temperature of the surface. The variation of $B(\lambda, T)$ for selected temperatures is depicted in Figure 2.1. At any wavelength, the emitted radiation increases with temperature and the blackbody curve shifts to the shorter wavelengths. The wavelength (λ_{peak}) at which the radiated power is at peak for a given temperature is given by Wien's displacement law as follows:

$$\lambda_{peak} = \frac{2897.8}{\mathrm{T}} \,\,\mu\mathrm{m} \tag{2.2}$$



Figure 2.1: The variation of the blackbody emissive power as a function of temperature [8].

2.2 The Solar Irradiance

The solar radiation spans the ultraviolet to infrared sections of the electromagnetic spectrum. Figure 2.2 shows the spectral distribution of the solar energy per unit area per unit time as received outside the atmosphere (also known as air mass 0 or AM0) and at sea level with the sun being at an angle of elevation of 42° (known as terrestrial or AM1.5). The extraterrestrial or AM0 solar irradiance spectra resembles the spectra of a blackbody at ~6000 K. The solar power density is 62 MW/m^2 at the sun's surface and is reduced to 1353 W/m^2 at the top of Earth's atmosphere. For the standard terrestrial solar spectrum or AM1.5, the integrated solar irradiance is defined to be 1000 W/m^2 . In this study, the AM1.5 solar irradiance is used to convert the incident power density to solar concentration factor.



Figure 2.2: Comparison of the extra-terrestrial (AM0) solar spectrum with the 6000 K blackbody spectrum and with the standard terrestrial (AM1.5) spectrum [9].

2.3 Radiative Properties

A natural body surface always radiates energy less than a blackbody at the same temperature. The emissivity (ϵ) of a surface is defined as the ratio of the thermal radiation emitted by the surface at a given temperature to the radiation emitted by a blackbody at the same temperature [8]. The value of ϵ is always between 0 and 1. ϵ of a surface is not a constant and varies with temperature and wavelength. ϵ =1 for a blackbody at all wavelengths. When radiation incidents on a surface, part of

it is reflected, part of it is absorbed, and the remaining part is transmitted. The fraction of incident radiation absorbed by the surface is called the absorptivity (α); the fraction reflected is called the reflectivity (ρ), and the fraction transmitted is known as transmissivity (τ). The first law of thermodynamics suggests that the sum of the reflected, absorbed, and transmitted radiation energy is equal to 1, or

$$\rho + \alpha + \tau = 1 \tag{2.3}$$

For an opaque surface, $\tau=0$, and thus $\alpha+\rho=1$. This is an important relationship as it allows to compute the surface α for an opaque surface by measuring the surface ρ . For a body at thermal equilibrium, the net heat transfer must be zero, which means the radiation emitted by the body is equal to the radiation absorbed by it. This results in the following relationship.

$$\varepsilon(T) = \alpha(T) \tag{2.4}$$

In this dissertation, the terms "absorptivity" and "emissivity" are used interchangeably.

2.4 Photovoltaic Conversion

Photovoltaic conversion occurs at the last stage of a STPV system to convert the thermally radiated photons from the emitter into electricity. TPV cells are an important component of STPV systems and should be chosen carefully to achieve an optimal system conversion efficiency. An optimal bandgap of the TPV cells is determined by the thermal emission spectrum, which in turn is controlled by the emitter temperature and the spectral characteristics of the emitter surface. The optimal operating temperature for an emitter is one for which the blackbody peak lies just above the bandgap of the TPV cell. Low bandgap cells (<1 eV) are preferred because they require lower operating temperatures (<1800 K) for the emitter [10]–[13]. Silicon (Si), which is commonly used in conventional PV cells, has an indirect bandgap of 1.12 eV or λ_{BG} = 1.11 µm, and is regarded

high for TPV applications. For a Si-cell based STPV system, the optimal operating temperature would be ~2600 K, which is quite high. For TPV conversion, Germanium (Ge), Gallium Antimonide (GaSb), and Indium Gallium Arsenide Antimonide (InGaAsSb) cells are of considerable interest due to their low λ_{BG} . Figure 2.2a shows the optimal emitter temperature required for a STPV device using different bandgap TPV cells. In this study, GaSb based cells are used for TPV conversion. The impact of the STPV temperature on the conversion efficiency of GaSb TPV cells is illustrated in Figure 2.2b. The blackbody power density at temperatures 1100 K, 1400 K, and 1700 K are shown along with the bandgap wavelength (λ_{BG}) of GaSb. With increasing temperature, the overall radiated power per unit area increases and the peak of the radiation curve shifts towards shorter wavelengths, as described before. Because only photons having wavelengths less than λ_{BG} can be converted to electricity, the maximum thermal-toelectrical conversion efficiency is limited by the fraction of the total radiated power that is below λ_{BG} . For a blackbody source at 1700 K, the maximum theoretical efficiency of a GaSb TPV cell is only 25.6%. Clearly, a blackbody emitter is not an ideal choice for STPV systems as it radiates a significant fraction of energy above λ_{BG} , thereby highlighting the critical role of spectrally selective emitter for boosting the system efficiency.



Figure 2.1: (a) Optimal STPV operating temperature for different bandgap STPV cells. (b) Spectral distribution of a blackbody radiation at temperatures 1100 K, 1400 K, and 1700 K, and its relevance to the conversion efficiency of a GaSb TPV cell.

2.5 Principle of STPV Operation

STPV systems can be realized in a variety of geometric configurations. Two most common architectures are planar and cylindrical arrangements. In a cylindrical STPV arrangement, the thermal emitter is in a shape of a cylinder and is surrounded by another larger cylindrical area tiled with small size PV cells. While a cylindrical configuration allows for a better control of the emitter area and improved radiative view factor between the emitter and PV cells, cylindrical STPV systems are more complex to fabricate [5]. On the other hand, the planar STPV systems are much simpler and offer less constraints on the PV cell area [12]. This dissertation focusses on the design and optimization of a planar STPV system.

A layout of a typical planar STPV system is shown in Figure 2.1. Unlike conventional solar photovoltaics, STPV utilizes concentrated solar radiation, which is absorbed and reemitted as thermal radiation towards a solar cell through a thermally coupled absorber and emitter pair. Most of the efficiency gain of STPV arises from the spectral control in the absorber/emitter structure that absorbs the broadband sunlight maximally and convert it into a narrowband thermal emission

tuned for the solar cell. The solar cells that are used to convert thermal radiation into electricity are often referred as thermophotovoltaic (TPV) cells. A selective spectral filter placed in between the emitter and the solar cell reflects the sub-bandgap photons back to the emitter for recycling. An infrared (IR) reflector or heat shield can also be installed on the absorber side to minimize the thermal radiation loss from the absorbing surface [14]. Effective recycling of the unused thermal radiation greatly enhances the system efficiency. The high incident power density results in thermal stress on the TPV cells. Therefore, a thermal management system, usually water-cooling, is implemented in STPV to keep the solar cells at room temperature (300 K).



Figure 2.3: Layout of a typical planar STPV system

2.6 Spectral Control Elements

Spectral control elements consist of thermally coupled absorber and emitter surfaces. They are essential in STPV systems for precise control of the absorption and emission of light needed to achieve high efficiency. A good absorber should efficiently absorb the broadband solar radiation, and meanwhile, exhibit low emittance at longer wavelengths to suppress re-radiation at the STPV

operating temperature. On the emitter side, the blackbody radiation spectrum must be narrowed to minimize the transmission and thermalization loss in TPV cells. An ideal emitting surface must have high emittance in the wavelength range matching the spectral response of the TPV cell, and low emittance beyond the bandgap wavelength (λ_{BG}) of the cell as well as far below λ_{BG} . An additional desired feature of the selective emitter is to have adequate bandwidth of thermal emission above the bandgap so that the TPV conversion would produce sufficiently high output power. Figure 2.4 shows absorbance spectra of ideal absorber (blue) and emitter (green) for a STPV system operating at 1700 K along with the blackbody radiation curve (magenta) and the normalized AM1.5 solar spectra (black). The overlap between the solar energy spectra and the thermal emission indicates that a perfect absorber is not feasible. An optimization of absorber- and emitter-side cut-off wavelengths is therefore required to maximize both the net accumulated spectral flux (Φ =absorbed solar energy-radiation loss) by the absorber [15] and the in-band thermal emission radiated toward the TPV cells. Besides, thermal stability is an important factor to consider when designing a spectral control element. Rare-earth elements like erbium, thulium, and ytterbium, and refractory metals, such as tungsten (W), molybdenum (Mo), and Tantalum (Ta), are promising materials for fabricating a selective absorber/emitter because of their high melting point and good intrinsic selective emission properties suitable for STPV applications [5]. Many techniques have been proposed and applied to achieve selective absorptivity for STPV absorbers and emitters and are reviewed in Chapter 3.



Figure 2.4: Normalized solar irradiance spectra at AM1.5 and a 1700 K blackbody spectra along with the spectral response of ideal absorber and emitter surfaces suitable for GaSb TPV cells.

2.7 Energy Flow in a STPV System

The flow of energy within a STPV system and various types of loss mechanisms occurring at different stages are shown in Figure 2.5. The concentrated solar power is converted into heat at the absorber side. The emitter, which is thermally coupled to the absorber, re-emits the heat at tailored wavelengths toward TPV cells. The thermally radiated photons with energy above the bandgap of the cells are absorbed to generate electricity at the output of the TPV cells. A fraction of the incident solar radiation is lost during the solar-to-thermal energy conversion process due to reflection and re-emission at the absorber. A certain amount of heat energy is lost via conduction through the support system incorporated for the absorber/emitter structure. Depending upon the extent of vacuum conditions, some convective heat loss may also occur in the system. Part of the radiation emitted by the emitter is not intercepted by the cells and is lost, which is referred to as

cavity loss. Among the thermal radiation from the emitter, only high-energy photons ($E>E_{BG}$) contribute to the electrical power at the output. Within TPV cells, conversion losses occur due to reflection, electron-hole recombination, thermalization, and non-ideal optical/electrical performance of the PV cell [16]. The system-level STPV efficiency is derived as the ratio of the electrical output power to the incident power.



Figure 2.5: Flow of energy within a STPV system.

Chapter 3: : Literature Review

3.1 Spectrally Selective Surfaces

The first TPV energy conversion device was built by Dr. Henry H Kolm [17] in 1956 at MIT's Lincoln Laboratory using a Coleman camping lantern as the thermal radiator and a silicon solar cell for PV conversion. The efficiency was poor because of the spectral mismatch between the thermal emission profile and the solar cell spectral response. A next key step towards improving the TPV conversion efficiency was the conceptual development of selective emitters that offer solar cell matched spectral emission than a blackbody.

In STPV systems, spectral selectivity is essential on both absorbing and emitting surfaces. A selective absorber is required at the input stage of the STPV system to absorb the maximum portion of the incident solar energy and convert it to heat. Because a good absorber is a good emitter too, a main challenge in designing a selective absorber is that it maximally absorbs the broadband solar irradiation and limits the thermal emission at the same time. Therefore, a selective absorber suitable for STPV systems should exhibit high absorptance around the peak of AM1.5 solar spectrum, and a very low emittance at infrared wavelengths. Spectral selectivity on the emitter side is also essential to maximize the thermal emission of photon with energies above the bandgap of the cell, while suppressing the emission of low-energy photons [11]. There are a variety of designs reported for selective surfaces suitable for STPV applications, including metal-dielectric composites [18]–[20], photonics crystals [21]–[23], rare-earth materials [24], [25], nanotube arrays [26], [27], nanoparticles [28], [29], and textured surfaces [30]–[32]. All of these designs utilize nanometer-scale structures that create interference effects to photons of wavelengths that are comparable to the sizes of these features. A more comprehensive review and

comparative analysis of the different selective surfaces for STPV applications is provided by Ungaro et al. [12], Gupta et al. [33], and Zhou et al. [11].

A selective emitter with abrupt cut-off at λ_{BG} is not feasible to fabricate and there are always some parasitic thermal losses, especially in the mid- and far-infrared. A spectral filter that allows transmission of photons with $\lambda < \lambda_{BG}$ and reflects all sub-bandgap photons back to emitter can further improve the system efficiency. Previous studies have reported resonance and plasmainterference filter structures based on semiconductors and transparent conducting oxides as potential edge filters for photon recycling in STPV systems [34]–[36]. Alternatively, re-utilization of sub-bandgap photons can also be achieved using metal reflectors at the back interface of TPV cells. Recently, Omair et al. (2018, 2019) reported 94% sub-bandgap reflectivity achieved by utilizing the photovoltaic band-edge as spectral filter and incorporating a rear gold reflector in a lattice-matched In_{0.53}Ga_{0.47}As TPV cell. An alternative approach of harvesting the sub-bandgap photons is by utilizing a multi-junction TPV cell structure. For example, Bendelala et al. [37] proposed a high-efficiency TPV system comprising of a meta-material film based selective emitter coupled to an InAs/GaInAsSb tandem cell, with a theoretical maximum thermal-to-electrical conversion efficiency of ~41% at 1773 K based on simulation.

3.2 TPV Cells

As described in Chapter 2, the selection of TPV cells for STPV applications is limited by the operating temperature of the selective emitter. TPV cells should be chosen such that the wavelength of the peak emission of a blackbody at the operating temperature matches with the bandgap of the material used for the TPV cells. Si with a bandgap of 1.12 eV is not suitable for TPV system operating below 1700 K, because the peak of the thermal radiation does not overlap with the Si band edge. Ge is an excellent alternative to Si due to its low bandgap (0.66 eV), but

based on previous studies, it showed a poor conversion efficiency due to very low open-circuit voltage [38], [39]. GaSb for its low bandgap energy of 0.72 eV has been extensively studied for use in STPV systems as well as in tandem solar cells [40]–[43]. Compared to Ge and Si, GaSb provides several advantages, such as a high fill-factor of 0.65, external quantum efficiency (EQE) reaching over 0.8, and efficiencies as high as 30%, assuming 100% recycling of the sub-bandgap photons [44]–[46]. An output power density of 2 W/cm² under the illumination of a blackbody radiation at 1500 K was reported by for an optimized design of a Heterojunction N+ on P GaSb thermophotovoltaic (TPV) cell [45]. InGaAsSb based TPV cells with a low bandgap of 0.5 eV have also been reported with EQE exceeding 60% and efficiency up to 30% [13], [47]. An advantage of using the InGaAsSb cells is that they can be used with the thermal radiators operating at a lower temperature of ~1200 K. This dissertation will focus on the use of GaSb TPV cells for both the theoretical and experimental studies due to their commercial availability and a reasonable conversion efficiency.

3.3 STPV Systems

Previous thermodynamic simulation studies predicted overall conversion efficiencies around 45% for less idealized STPV systems [4], [16], [22]. But, to date no experimental demonstration of a STPV system has been put forth with efficiency reaching these levels. Most of the early designs were based on cylindrical configurations utilizing a centered radiator surrounded by a large cavity made of TPV cells (Datas and Algora, 2012; Vlasov et al., 2007; Yugami et al., 2000). Owing to low radiative view factor (VF) between the emitter and TPV cells, lack of robust cooling units to prevent overheating of the TPV cells, high optical concentration losses, inefficient thermal extraction, and low area-ratio of emitter to TPV cells, their reported efficiency was poor (<1%). In 2014, a more robust and efficient STPV system using a vertically aligned multi-walled carbon

nanotube blackbody absorber and a 1-D Si/SiO2 photonic crystal as a selective emitter was built by Lenert et al. [26]. This system was a compact planar design that could be operated at much lower optical concentration, thereby enabling significant reduction in the optical losses compared to the previous designs [7], [48]. A narrow-bandgap InGaAsSb TPV cell (0.55 eV) was used that allowed efficient operation at lower system temperature (1285 K). The system was tested under simulated solar conditions and the efficiency of 3.2% was reported. Low conversion efficiency of the InGaAsSb TPV cell was one of the key limiting factors in their STPV design.

Ungaro et al. [31] demonstrated a high efficiency STPV system utilizing nanostructuresbased selective absorber/emitter fabricated on a W substrate and GaSb cells. The reported efficiency was 6.2% at ~1700 K. Another high-efficiency planar STPV configuration using GaSb cells was presented by Kohiyama et al. [14] with a measured system efficiency of 5.1%. They utilized multilayer coatings of Molybdenum (Mo) and Hafnium oxide (HfO2) on a Mo substrate for constructing a selective absorber/emitter structure. The highest STPV system efficiency reported so far was achieved by pairing a tandem plasma-interference optical filter with a 1-D Si/SiO2 photonic crystal based selective emitter [51]. The filter was engineered to reflect 80% of the sub-bandgap photons back to the emitter while allowing the in-band photons to pass through. Using an InGaAsSb cell, the reported system efficiency was 6.8%. Table 1 summarizes the key features of the selected STPV published works before [14], [26], [31], [51]. A more detailed review of previous experimental and simulated STPV systems was discussed by Gupta et al. [52]. Recently, Ni et al. [53] presented a theoretical analysis of a low-concentration STPV system utilizing a spectrally selective five-layer metafilm (SiO₂, Si₃N₄, W, SiO₂, and W from top to bottom) absorber/emitter structure paired with an InGaAsSb TPV cell. Their analysis showed 50% emission loss from the absorbing surface and the overall STPV system efficiency of 7.1% at 50
suns. The study discussed the optimization of the metafilm structure to achieve >10% system efficiency under 50 suns, but it hasn't been tested via experimental procedure.

Table 3.1: Ke	y features of selected	experimental STPV	systems reported in	[14]	, [26]	, [31]	[51]
		1	2		2 E		

Work	Emitter structure	STPV temperature	TPV cells	System efficiency
Lenert et al. (2014)	Si/SiO ₂ stack	1285 K	InGaAsSb	3.2%
Ungaro et al. (2015)	W with Si_3N_4 thin film	1700 K	GaSb	6.2%
Kohiyama et al. (2016)	Mo/HfO ₂ nanostructures	1640 K	GaSb	5.1%
Bierman et al. (2016)	Si/SiO ₂ stack	1273 K	InGaAsSb	6.8%

Chapter 4: STPV System Modeling and Optimization

STPV is a complex system comprising of a number of elements influencing the overall conversion efficiency. A comprehensive theoretical analysis using both optical modeling and thermodynamic simulation is necessary to fully characterize the performance of an STPV system. This chapter formulates optical and thermodynamic models to simulate the performance of a practical STPV system that was fabricated and tested in this study.

4.1 Optical Modeling of Surface Emissivity

The optical response of an emitting surface composed of a multilayer metal-dielectric stack can be modeled using a standard transfer matrix method (TMM). The TMM is based on Fresnel equations and offers a computationally efficient means for computing reflectance, transmittance, and absorption of a light incident on a multilayer planar stack, provided that the medium in each layer of the stack is isotropic and homogenous with a spectrally dependent complex relative permittivity [33], [54], [55]. Using the Fresnel equations, a 2x2 transfer matrix can be defined for all layers in the stack. These matrices are multiplied together to obtain the system transfer matrix that allows to compute the overall reflection and transmission of light through the system. For an optically opaque structure, such as the tungsten substrate in this case, the emissivity or absorptivity of a surface can be simply modeled as (1-reflectivity). Numerous researchers [4], [56], [57] have successfully implemented the TMM for designing multilayer selective surfaces suitable for TPV applications.

The spectral absorptivity of the $Si_3N_4/W/Si_3N_4$ stack employed in this study was also modeled using TMM implemented in Python. The required optical constants, refractive index (n) and extinction coefficient (k), for W and Si_3N_4 at room temperature (300 K) were obtained from literature [58], [59]. For Si_3N_4 , k is assumed to be zero between 0.5-5.5 µm, which is the range of simulation used in this study. Figure 4.1 shows the comparison between the simulated reflectance spectra (using TMM) of tungsten with the measured spectra using a Varian Cary 5E Spectrophotometer. The two spectra show a good agreement.



Figure 4.1: Simulated and measured reflectance spectra of a polished tungsten surface.

4.2 Thermodynamic Modeling of STPV System

A complete thermodynamic model was formulated and developed using the Interactive Data Language (IDL) programming platform to analyze the flow of power at multiple stages of the STPV system.

4.2.1 Power balance at thermal equilibrium

When a concentrated solar radiation is incident on the absorber surface, the temperature of the absorber/emitter structure increases until thermal equilibrium is reached. For a given incident

concentrated power (P_{in}), the equilibrium temperature can be computed by solving the following equation.

$$P_{in} - P_{ref} - P_{rad,abs}(T) - P_{rad,side}(T) - P_{conv}(T) - P_{cond}(T) - P_{rad,emit}(T) = 0$$
(4.1)

where P_{ref} is the amount of power reflected off the absorbing surface, $P_{rad,abs}(T)$ is the thermally radiated power from the absorbing surface, Prad, side(T) is the power loss due to radiation from the 4 sides of the W substrate, $P_{conv}(T)$ is the convective power loss, $P_{cond}(T)$ is the conduction loss due to support systems, and Prad, emit(T) is the net radiant flux emitted from the emitter surface. The thermal radiation emitted from a surface can be computed from Planck's function and by knowing the spectral emissivity of the surface. In our simulation, the emissivity of the involved surfaces is simply assumed to be (1-Reflectivity). The reflectance spectra of polished W substrate and the metal-dielectric stack were derived using the TMM simulation. Prad. side is computed in the similar way using the emissivity of W. P_{rad.abs} consists of two components: one radiated from a highly emissive microtextured area (A_{abs}=0.64 cm²), and second from the inactive or non-textured W area (5.81 cm^2) . P_{conv}(T) is simulated using equations for natural convection above a horizontal surface as provided in literature [60]. The conduction loss (P_{cond}) from support was computed using fin approximation equations as described by A. Lenert et al. [26]. Finally, the radiant flux power Prad, emit from the emitter surface was estimated using Planck's blackbody equation and the spectral emissivity of the surface.

4.2.2 Absorber selectivity and optimization

When the concentrated solar radiation is incident on the absorber surface, a part of the incident solar energy is lost due to the reflection from the absorber. A near-blackbody absorber, such as an array of vertically aligned multi-walled carbon nanotubes [26], can offer high absorbance over a broad range of the solar spectrum. Because a good absorber is a good emitter too, there will be a

significant radiation loss from the absorber as it reaches high temperatures. Therefore, another requirement for an efficient absorber is to have low emittance, especially in near-infrared wavelengths, where the blackbody radiation is higher for STPV operating temperatures. A selective absorber with an extremely high absorbance near the peak of AM 1.5 spectrum, and low emittance (or absorbance) at infrared wavelengths can greatly enhance the absorber-to-emitter thermal extraction, which is desirable for a high-efficiency STPV system [11], [14]. Figure 4.2a shows an example absorbance spectrum (in blue) of an ideal absorber for a STPV system operating at 1700 K along with the blackbody radiation curve (magenta) and the normalized AM1.5 spectrum (black). The overlap between solar energy and the thermal emission indicates that a perfect absorber is not feasible. An optimization of absorber-side cut-off wavelength ($\lambda_{abs-cut}$) is required to maximize the net accumulated spectral flux (Φ =absorbed solar energy-radiation loss) by the absorber [15]. The optimal value of $\lambda_{abs-cut}$ is determined by the absorber operating temperature and the incident solar concentration factor (C_x). Higher operating temperatures require a lower λ_{abs} cut because of the increased thermal radiation at shorter wavelengths, and vice-versa, in accordance with the Wein's displacement law. $\lambda_{abs-cut}$ for the absorber equilibrium temperatures of 1400 K and 1700 K at a constant Cx=100 are shown in Figure 4.2b. Similarly, the optimal $\lambda_{abs-cut}$ shifts towards longer wavelengths for higher C_x values, provided that the equilibrium temperature remains the same. This is illustrated in Figure 4.2c. Thus, it is crucial to consider the operating temperature and available solar concentration to design and fabricate a selective solar absorber with the highest thermal extraction efficiency.



Figure 4.2: Normalized values of AM1.5 solar spectra (black), blackbody radiation curve at 1700 K (magenta), and the absorptivity of an ideal absorber (blue step function). (b) Net radiation flux collected by an absorber as a function of cut-off wavelength. The optimal cut-off wavelength ($\lambda_{abs-cut}$) are also shown for 1400 K (dashed blue line) and 1700 K (solid red line) equilibrium temperatures acquired at a constant C_x=100. (c) Same as (b) but for a constant equilibrium temperature of 1700 K at C_x=100 (red) and C_x=300 (blue).

4.2.3 Emitter selectivity and optimization

For a blackbody emitter at 1700 K, only 26% of the emitted spectrum is above the GaSb cell bandgap (Chapter 2). Clearly, a blackbody is not an ideal choice for an STPV emitter, unless an effective recycling scheme is incorporated to reflect unconvertible photons back to the emitter.

Otherwise, spectral selectivity is required for an emitter to suppress the longer wavelength photons $(\lambda > \lambda_{BG})$ beyond the TPV cell bandgap, while enhancing the emission of photons with energy above the bandgap ($\lambda < \lambda_{BG}$). Besides, thermal stability is an important factor to consider when designing a spectral control element. As discussed before, rare-earth elements like erbium, thulium, and ytterbium, and refractory metals, such as tungsten (W), molybdenum (Mo), and Tantalum (Ta), are promising materials for fabricating a selective absorber/emitter because of their high melting point and good intrinsic selective emission properties suitable for STPV applications [5], [12]. Another key aspect of designing a selective emitter is the bandwidth of thermal emission. One would desire that the selective emitter has adequate bandwidth of thermal emission above the bandgap so that the TPV cells would produce maximum output power. However, increasing the bandwidth far above the bandgap may result in increased thermalization loss that impairs the TPV conversion efficiency (η_{TPV}). The optimal bandwidth of thermal emission to maximize η_{TPV} can be derived using the external quantum efficiency (EQE) data of the TPV cells. The GaSb cell EQE is shown in Figure 4.3a (courtesy of JX Crystals Inc.). The right edge of the EQE plot represents λ_{BG} . The simulated values of thermalization loss and η_{TPV} as a function of the selective emitter bandwidth ($\Delta\lambda$) are shown in Figure 4.3c. The spectral emittance is assumed to have a unit step function response with its right edge being fixed at λ_{BG} . $\Delta\lambda$ is varied by shifting its left edge towards shorter wavelengths. The emitter temperature is considered to be 1700 K in the simulation. The thermalization loss (red curve) increases with increasing the bandwidth until the bandwidth surpasses the left edge of the EQE curve. The optimal bandwidth of selective thermal emission for maximum η_{TPV} of the GaSb cells is estimated to be around 400 nm.



Figure 4.3: (a) EQE plot for GaSb TPV cells purchased from JX Crystals along with a varying bandwidth step function. (b) Thermalization loss and η_{TPV} as a function of emitter bandwidth computed at 1700 K emitter temperature. The bandwidth corresponding to the peak η_{TPV} is shown by a dashed vertical line.

An ideal selective emitter with a unit step response for spectral emittance is not possible to fabricate in practice. So, for a practical selective emitter, there are two figures of merit that are commonly used to assess its performance. They are spectral selectivity (η_{sel}) and in-band emissivity ($\epsilon_{in-band}$), which are defined by Equation 4.2 and Equation 4.3, respectively.

$$\eta_{sel} = \frac{\int_0^{\lambda_{BG}} \varepsilon(\lambda)B(\lambda,T)d\lambda}{\int_0^\infty \varepsilon(\lambda)B(\lambda,T)d\lambda}$$
(4.2)

$$\varepsilon_{in-band} = \frac{\int_0^{\lambda_{BG}} \varepsilon(\lambda)B(\lambda,T)d\lambda}{\int_0^{\lambda_{BG}} B(\lambda,T)d\lambda}$$
(4.3)

where $\varepsilon(\lambda)$ is the emissivity of the selective emitter, $B(\lambda, T)$ is Planck's blackbody function. For optimal thermal-to-electric conversion, it is important that the thermal emission from the emitter matches the spectral response of the TPV cells (high η_{sel}) and the emitted radiant power below λ_{BG} is maximum (high $\varepsilon_{in-band}$). The maximum value of η_{sel} and λ_{BG} is 1.

4.2.4 Thermal energy extraction efficiency and geometry optimization

High-efficiency STPV systems require a high absorber-to-emitter heat extraction rate. Thermal extraction efficiency (η_e), which is the ratio of the power emitted by the emitter to the power incident on the absorber side, is governed by both spectral and geometric properties of the absorber and emitter [20]. Suppressing the reflection and emission losses from the absorber surface, and meanwhile, maximizing $\varepsilon_{in-band}$ of the emitter surface can yield in a high η_e value, which is given by the following equation.

$$\eta_e = \frac{P_{rad,emit}}{P_{in}} \tag{4.4}$$

High absorbance of the absorber also results in high emission losses from the absorbing surface. Besides spectral selectivity, geometric optimization can also help in reducing the absorber-side emission losses. This is usually done by keeping the absorber area small compared to that of the emitter [7], [20], [61]. The geometric control of η_e is, therefore, defined by the emitter-to-absorber area ratio (AR).

4.2.5 Cavity loss

Owing to a finite spacing between the emitter and TPV cells, not all the radiation leaving the emitter surface is intercepted by the cells. This is referred to as cavity loss. A radiative view factor (VF), which is defined as the fraction of the radiation leaving the emitter that strikes the cells, can be computed based on the geometry and orientation of the two surfaces. Cavity loss is computed as (1-VF). The cavity loss (expressed in %) for two square surfaces as a function of the separation distance (d) between them is shown in Figure 4.4. The cavity loss increases exponentially with d. For d=1 mm, the cavity loss is $\sim 8\%$ (VF=0.92). The cavity loss increases to 50% when d=10 mm.

VF is a crucial parameter to be considered in the design of a high efficiency STPV system, and should be maximized as possible.



Figure 4.4: Cavity loss as a function of separation distance between two equal-area square parallel plates.

4.2.6 Photon recycling

In real STPV systems, the practical implementation of any spectral selectivity exhibits nonidealities [15] that prohibit from achieving a zero emittance above $\lambda_{abs-cut}$ for the absorber side and above λ_{BG} for the emitting surface. In both cases, the emission of the longer wavelength photons leads to increased thermal radiation loss within the STPV system. A significant improvement in the system efficiency can be achieved via recycling schemes that involve reflecting these unused photons back to the absorber/emitter. On the absorber side, a heat shield made of a material with high infrared reflectivity, such as gold (Au), can be installed to reflect the thermal radiation back to keep the absorber at high temperatures. Figure 4.5a shows the emittance of a W surface alone (black curve) and its effective emittance (ϵ_{Eff} in green curve) in the presence of a Au reflector placed at 1mm distance from the absorber surface modeled using Equation 4.5 [14], [15].

$$\varepsilon_{Eff} = \left(\frac{1}{\varepsilon_{W}} + \frac{1}{1 - \varepsilon_{Au}}\right)^{-1}$$
(4.5)

where ε_W and ε_{Au} are the spectral absorptivity or emittance of W and Au, respectively. The installation of the Au shield can suppress ~90% of thermal radiation loss from the W absorber at 1700 K. The advantage of using the Au reflector is greater for higher temperatures because the peak of the thermal radiation shifts towards shorter wavelengths (dashed blue and magenta curves in Figure 4.5a) where the spectral emissivity of W increases up to 0.5.

On the emitter side, one would prefer all low-energy photons below the bandgap are reflected back to the emitter. A selective window filter that is transmissive to in-band radiation and highly reflective at wavelengths $>\lambda_{BG}$ placed in between the emitter and TPV cell can serve this purpose. Several resonance and plasma-interference filter structures based on semiconductors and transparent conducting oxides as potential edge filters have been reported in previous studies for photon recycling in STPV systems [34]–[36]. Recycling of sub-bandgap photons can also be achieved using metal reflectors at the back interface of TPV cells. A recent study [62] reported achieving a 95% average reflectivity for below-bandgap photons by incorporating a rear gold reflective mirror in a lattice-matched In_{0.53}Ga_{0.47}As TPV cell. The spectral reflectance of the GaSb TPV cells purchased from JX Crystals Inc. is shown in Figure 4.5b. The blue curve represents the area-weighted surface reflectance (due to the active area of the cell and the silver grid bars) measured using the Varian Cary 5E Spectrophotometer. After accounting for the reflectance from the silver grid bars, the active area of cells has maximum absorption (~5% reflectance) near 1.4

 μ m (green curve), where the spectral response of the cell is at peak. At sub-bandgap wavelengths (above λ_{BG}), these cells can offer an average reflectivity of ~30% for photon recycling.



Figure 4.5: (a) Effective absorptivity (green) of a W-Au arrangement is significantly lower than that of plain W (black) at shorter wavelengths due to the high infrared reflectivity of Au (red curve). The benefit of using the Au heat shield is larger at higher temperature due to the blackbody radiation curve (blue for 1000 K and magenta for 1700 K) shifting towards shorter wavelengths where the emissivity of W is greater. (b) GaSb cell reflectance (blue) measured using the Varian Cary 5E Spectrophotometer. The reflectance of only the active cell area is shown in green. The dashed vertical line represents the λ_{BG} for GaSb.

4.2.7 STPV system efficiency

The overall STPV system efficiency (η_{STPV}) is modeled as:

$$\eta_{STPV} = \eta_e \cdot \eta_{sel} \cdot \eta_{PV} \tag{4.6}$$

where η_e , η_{PV} , and η_{sel} are the thermal extraction efficiency of the absorber, the photovoltaic conversion efficiency of the GaSb cell, and the spectral conversion efficiency of the selective emitter, respectively.

4.3 GaSb Solar Cells

The short-circuit current density (J_{sc}) for the GaSb TPV cells used in this study is modeled by integrating the photon flux absorbed by the TPV cell across the wavelengths less than λ_{BG} . The

EQE data required for computing J_{sc} was provided by JX Crystals. The expression for computing J_{sc} is provided below.

$$J_{sc} = q \times VF \times \int_0^{\lambda_{BG}} \frac{\lambda}{hc} B(\lambda, T) \cdot \varepsilon(\lambda) \cdot EQE(\lambda) d\lambda \quad A/cm^2$$
(4.7)

where $hc/\lambda =$ is the photon energy and $\varepsilon(\lambda)$ is the spectral emissivity or absorptivity of the emitter. The reverse saturation current density (J₀), bandgap, and open circuit voltage (V_{OC}) for the GaSb cells are dependent on the cell temperature (T_{Cell}) and are determined using the empirical expressions provided by Fraas et al. [41].

$$J_0 = (1.84 \times 10^{-3}) T_{Cell}^3 \exp\left(-\frac{E_{BG}}{kT_{Cell}}\right), \ A/cm^2$$
(4.8)

$$E_{BG} = 0.813 - 6 \times 10^{-4} \frac{T_{Cell}^2}{T_{Cell} + 265}$$
(4.9)

$$V_{OC} = (kT_{Cell}/q) \ln[\frac{J_{SC}}{J_0} + 1],$$
 (4.10)

Equations 4.8 through 4.10 indicate that J_0 increases with TPV cell temperature, thereby reducing V_{OC} and overall conversion efficiency of the cell. Therefore, it is important to maintain the operating temperature of the GaSb cells to room temperature for optimal performance.

4.4 STPV System Model Description and Parameters

During simulation formulation, there are certain parameters, such as absorber and emitter areas, bandgap of TPV cells, radiative view factors, vacuum conditions, etc., that are set fixed throughout the simulation process. It is relevant to discuss those parameters in this section. The STPV system built and tested in this study consists of a microtextured absorbing surface and a multilayer metal-dielectric (Si₃N₄/W/Si₃N₄) coated selective emitter fabricated on opposite sides of a 25.4 x 25.4 x 0.5 mm polished tungsten substrate. The textured absorber area is only 0.64 cm², while the emitting surface utilizes the full 6.45cm² area of the emitter side. The absorptivity of the textured surface was measured using an integrating sphere setup that is described later. An Au heat shield is

installed on the absorber side to suppress the thermal radiation loss from the non-active region of the absorber area. The emitter was supported on two silica rods with thermal conductivity of 1.38 W/mK. The bandgap of GaSb cell is 0.72 eV or $1.7 \mu \text{m}$. The finite spacing (<1.5 mm) between the emitter and cell results in a radiative VF of 0.91. The vacuum condition is set to 80 mTorr and the TPV cell temperature is assumed to be 300 K. The schematic of the STPV system used in this simulation study is shown in Figure 4.6. Table 4.1 provides a list of various constant parameter values used in the simulation.



Figure 4.6: Schematic of the STPV system set up for the simulation.

Table 4.1. Summary of the unterent parameter	values used in the simulation.
Model parameter	Value
Absorptivity of micro-textured W based on measurements	0.92
Area of W substrate	6.45 cm^2
Micro-textured absorber area	0.64 cm^2
Non-textured absorber area	5.81 cm^2
Combined area of four edges of the substrate	0.51 cm^2
Thermal conductivity of the support	1.38 W/mK

Table 4.1: Summary of the different parameter values used in the simulation.

Emitting surface area	6.45 cm^2
TPV cell area	5.92 cm^2
Distance between heat shield and absorber	1.8 mm
Distance between emitter and TPV cells	1.5 mm
VF between emitter and TPV cells	0.91
Pressure inside the chamber	80 mTorr

4.5 Simulation Results

4.5.1 Thermal extraction vs AR

As discussed earlier, high-efficiency STPV systems require a high value for η_e , which can be achieved by implementing an optimal spectral selectivity while designing the absorber and emitter surfaces. Besides, geometric optimization can also significantly improve η_e by reducing the absorber-side emission losses. Figure 4.7 illustrates the dependency of η_e on AR for 3 cases: (a) both absorber and emitter are blackbody surfaces (red curve), (b) emitter is blackbody while absorber is spectrally selective with $\lambda_{abs-cut}=2.0 \ \mu m$ (blue curve), and (c) both absorber and emitter are blackbody with the inactive area of the absorber being shielded with an Au reflector. In each of these cases, the steady-state temperature of the absorber/emitter surfaces is assumed to be 1700 K. In a planar STPV design, the absorber and emitter share the same substrate. Usually, one side of the planar substrate serves as an absorber and the opposite surface as an emitter. For equal-area (AR=1) blackbody emitter and absorber, $\eta_e=50\%$ (red curve) as both the surfaces emit an equal amount of radiation (assuming the radiation losses from edges are negligible). The radiation loss from the absorber can be lowered by decreasing the absorber surface area or increasing AR. For an AR=10, ne increases to ~90%. For a planar STPV configuration, the physical dimensions of the absorber and emitter sides are likely the same as they use the common planar substrate. However, the active absorber area, which receives the concentrated solar radiation, can be limited to a smaller portion of the absorber side. The remaining or inactive area on the absorber side is required to have low emittance (ideally zero) to minimize radiation loss. The red curve in Figure 4.7 assumes that the radiation loss from the inactive area on the absorber side is zero for AR>1. This is not true in practice. In a real STPV setup, the inactive area is shielded with a heat reflector. This case is illustrated with the dashed black curve in Figure 4.7, where an Au-based heat reflector is used to shield the radiation loss from the inactive area. The value of η_e is little lower but comparable to the case where the inactive area has zero emittance. Significant improvement in η_e can be achieved at lower AR if the absorber features a spectral selectivity with $\lambda_{abs-cut}=2.0 \ \mu m$. This is because of the fact that at 1700 K, blackbody emits a significant fraction of radiation beyond 2.0 μm . The suppression of this radiation results in a greater value of η_e at lower AR values. The STPV system designed and fabricated for this dissertation study uses an optimal value of AR=10.



Figure 4.7: (a) Effect of Emitter-to-absorber area ratio (AR) on thermal extraction for a blackbody absorber and emitter (red), selective absorber (blue), and blackbody absorber with a gold heat shield.

4.5.2 Optimal selective emitter

A multilayer structure consisting of two layers of Si₃N₄ dielectric and a layer of W sandwiched in between is proposed as a selective emitter for this study. The optical response of the multilayer emitting surface was modeled using a standard transfer matrix method (TMM). The optical constants for W and Si₃N₄ required for the TMM simulation were obtained from the literature [58], [59]. A parametric sweep allowing the film thicknesses of the three nanolayers to vary with a 5 nm step size was run to derive the optimal thicknesses that would result in high η_{sel} and $\varepsilon_{in-band}$ so as to maximize the GaSb cell output. The spectral absorptivity of 12 such simulation cases is shown in Figure 4.8. Case 1 represents the absorptivity of plain W. The values of η_{sel} , $\varepsilon_{in-band}$, and emitted power density (P_{emit}) computed at 1700 K for all these cases are listed in Table 4.2. Tungsten exhibits an excellent η_{sel} (69.2%) but poor $\varepsilon_{in-band}$ (0.33). Based on the simulated reflectance spectra, the multilayer structure consisting of two 120 nm layers of Si₃N₄ and a 25 nm layer of W in between (Case 9 in Fig. 6 and Table 1) offers the combined optimal values of η_{sel} (~71%) and $\varepsilon_{in-band}$ (0.95), and thus chosen for this study.



Figure 4.8: Simulated absorptivity of multiple Si₃N₄/W/Si₃N₄ thin-film stacks aimed for achieving a high spectral selectivity emitter for GaSb TPV cells.

Case #	Emitter Design Si ₃ N ₄ /W/Si ₃ N ₄	η _{sel} (%)	E _{in-band}	$P_{rad, emit} (W/cm^2)$
1	Plain W	69.2	0.33	5.19
2	80 nm/10 nm/80 nm	73.4	0.91	15.02
3	80 nm/15 nm/80 nm	74.1	0.89	14.52
4	80 nm/20 nm/80 nm	74.6	0.85	13.80
5	85 nm/20 nm/85 nm	74.2	0.88	14.30
6	90 nm/25 nm/90 nm	74.3	0.86	14.03
7	100 nm/20 nm/100 nm	72.5	0.93	15.60
8	110 nm/25 nm/110 nm	72.3	0.93	15.63
9	120 nm/25 nm/120 nm	70.9	0.95	16.23
10	120 nm/30 nm/120 nm	71.9	0.92	15.53
11	130 nm/25 nm/130 nm	69.3	0.93	16.69
12	140 nm/30 nm/140 nm	68.9	0.93	16.31
13	160 nm/35 nm/160 nm	67.0	0.83	15.10

Table 4.2: η_{sel} , $\epsilon_{in-band}$, and P_{emit} computed for different emitting surfaces at T=1700 K.

Figure 4.9 shows the spectra of thermal radiation from a blackbody (dashed blue curve) and the Case 9 Si₃N₄/W/Si₃N₄ selective emitter (red curve) at 1700 K. A tungsten surface exhibits an excellent η_{sel} but poor $\varepsilon_{in-band}$. A blackbody emitter provides maximum in-band emission, but its spectral selectivity is only 25.6%. Compared to a bare W substrate, the radiant flux emitted by the Si₃N₄/W/Si₃N₄ surface is nearly 3 times greater. The peak of the thermal emission from the selective emitter matches very well with the peak of the EQE (black curve) of the GaSb cells.



Figure 4.9: Comparison of the spectral emissions from a blackbody (dashed blue), and the $Si_3N_4/W/Si_3N_4$ selective emitter (red) at 1700 K. The GaSb cell EQE is also shown in black curve.

4.5.3 Steady-state temperature vs incident light power

When a concentrated solar radiation is incident on the absorber surface, the temperature of the absorber/emitter structure increases until thermal equilibrium is reached. The required incident power to acquire a steady-state absorber/emitter temperature is determined by the system losses and net emission from the emitter. The simulated steady-state absorber/emitter temperature as a

function of the concentrated input power incident on the absorber surface is shown in Figure 4.10. The black curve shows a case of no photon recycling. For the same incident power, the STPV equilibrium temperature goes up with the installation of the gold reflector over the inactive region of the W absorber, as shown by the red curve. The combined effect of photon recycling due to the heat shield and the reflection off the GaSb cells is illustrated by the green curve. The simulation results show that the input solar concentration power required to achieve the steady-state temperature of 1700 K reduces from 165 W (2580 Sun) to 103 W (1610 Sun) due to the combined photon recycling from the Au reflector and TPV cells. The lowered energy budget at the steady-state temperature of operation is desirable as a lower solar concentration is easier to achieve from the practical point of view.



Figure 4.10: Steady-state STPV temperature as a function of incident power. Black curve represents a case of no photon recycling. Effect of the gold reflector over the inactive area of the absorber is shown in Red. Green curve shows the combined effect of photon recycling on both absorber and emitter sides.

4.5.4 System performance

Thermal management of the TPV cells is an important aspect of the STPV design. Figure 4.11 shows the degradation of the GaSb cell E_{BG} and V_{OC} as a function of the cell temperature derived using Equations 4.8, 4.9, and 4.10. A ~20% reduction in V_{OC} is expected if the cell temperature rises from 300 K to 360 K. For a STPV system with high output power density, air cooling may not be adequate because of its low heat transfer coefficients (<10 mW/cm²K), thus forcing to use active cooling systems to keep the cells at a reasonably low temperature [5].



Figure 4.11: Temperature dependence of E_{BG} and V_{OC} derived from Equations 4.8 through 4.10.

The modeled J_{SC} and V_{OC} for the GaSb cells at different emitter temperatures are provided in Figure 4.12. Results are shown for both a blackbody radiator (green curve) and the Si₃N₄/W/Si₃N₄ selective emitter (black curve). J_{SC} increases proportionally with the intensity of the incident illumination. According to Planck's law, the radiation power density scales at a rate proportional to the fourth power of the absolute temperature. As such, J_{SC} increases exponentially at higher radiator temperatures as the peak value increases in magnitude as well shifts toward the shorter wavelengths matching the EQE of GaSb cells. Similarly, V_{OC} also increases with the emitter temperature but is less sensitive because it is proportional to the natural logarithm of the incident illumination. J_{SC} and V_{OC} for the selective emitter are slightly lower than those for the blackbody emitter because the selective emitter has $\varepsilon_{in-band} < 1$.



Figure 4.12: GaSb cell (a) J_{SC} and (b) V_{OC} derived for a blackbody radiator and the $Si_3N_4/W/Si_3N_4$ selective emitter as a function of radiating substrate temperature.

The simulated peak output power density of GaSb cells for different radiating substrate temperatures is shown in Figure 4.13a. The overall STPV system conversion efficiency as a function of emitter temperature is depicted in Figure 4.13b. Black curve represents modeled efficiency for the no photon recycling case, whereas the blue curve is for the case with the photon recycling implemented using an Au-reflector for the absorbing side and considering the TPV cell reflectance into account. A noticeable improvement in the system efficiency can be seen by suppressing the parasitic heat losses in the conversion process. With increasing temperature, the thermal emission from the emitter not only increases but also exhibits a better spectral matching

with the EQE of the TPV cell, thereby resulting in an exponential growth in the TPV cell output and system efficiency.



Figure 4.13: (a) GaSb cell output power density for a blackbody emitter and the $Si_3N_4/W/Si_3N_4$ selective emitter as a function of the emitter temperature. (b) Modeled system efficiency as a function of the selective emitter temperature (black curve is for no photon recycling and blue curve is with photon recycling).

The modeled system efficiency at 1700 K is computed to be ~14%, and it drops to 9% in the absence of the photon recycling scheme that is implemented in the current system. The equivalent solar concentration corresponding to the STPV input power can be calculated assuming an incident solar power of 0.1 W/cm² (AM 1.5). The system efficiency of 14% is computed at an input solar concentration factor of 1610, which is within the practical limit and is achievable with Fresnel lens setup.

4.6 Conclusions

In this chapter, a combination of thermodynamic modeling and TMM simulation was used for a detailed-balance analysis of a practical STPV system using GaSb TPV cells. The study involved comprehensive analysis required for the design and optimization of spectrally selective surfaces that are essential components of high-efficiency STPV systems. Significance of determining the optimal emitter temperature, $\lambda_{abs-cut}$, AR, and emitter bandwidth for global system optimization

was discussed. The relevance of photon recycling on both the absorbing and emitting sides for achieving high η_e and η_{STPV} was investigated. A high-efficiency planar STPV system comprising a microtextured absorber and a Si₃N₄/W/Si₃N₄ coated tungsten selective emitter is designed and modeled. The desired thicknesses of the metal-dielectric layers for the optimal absorptivity spectra suitable for GaSb cells were derived using TMM simulations. A heat shield made of a gold foil was installed to suppress the back-radiation loss from the absorber side, and its effect on steady-state temperature, thermal extraction efficiency, and overall system efficiency was studied. The effect of AR on system performance was also investigated. The J_{SC} and V_{OC} of the GaSb cells were computed using the EQE data provided by the cell vendor and from the knowledge of the thermal emission spectra of the emitter. The $Si_3N_4/W/Si_3N_4$ structure consisting of two 120 nm layers of Si₃N₄ and a 25 nm layer of W was found to provide the most optimal emission spectra ($\eta_{sel} = -71\%$ and $\epsilon_{in-band} 0.95$) matching the EQE of the GaSb TPV cells. The overall system efficiency at 1700 K was modeled to be ~14%. Table 4.3 summarizes the optimized values of selected design parameters used in the simulation study for achieving $\eta_{STPV} = 14\%$ at 1700 K substrate temperature. Values of other system parameters are provided in Table 4.1. A part of the work presented in this chapter has been submitted to the Optics Express journal for publication [63].

Design parameter	Value	
AR	10	
$\eta_{_{SEL}}$	70.9%	
E in-band	0.95	
η _e	90%	
Temperature of TPV cells	300 K	
Reflectance of gold film (0.8-5 μ m)	0.98	

Table 4.3: Optimized values of selected design parameters to achieve 14% STPV system efficiency.

Chapter 5: Experimental STPV System

Utilizing the knowledge acquired from the simulation analysis presented in the previous chapter, a complete STPV system comprising a planar absorber/emitter structure and GaSb cells. was designed, fabricated, and tested. Tungsten is chosen for the absorber/emitter substrate due to its high melting point and good intrinsic optical properties suitable for STPV applications. The experimental system is described in detail in the following sections

5.1 GaSb Cells

The GaSb TPV cells used in this experiment were purchased from JX Crystals. Four square cells, with an area of 1.48 cm² each (total cell area is 5.92 cm²), were mounted on a copper substrate via reflow soldering. The cell mount was actively cooled using circulating water at 10°C. The cells have an anti-reflection coating on top to minimize the reflection near 1.4 µm. Based on the specification provided by JX Crystals, the EQE of these cells peaks near 1.5 µm [44]. The reflectance spectra (Figure 4.5b) of the TPV cell was measured using the spectrophotometer and was found to be $\sim 5\%$ (after accounting for the reflectance from the silver grid bars on the cells) near 1.4 µm, and up to 40% at sub-band wavelengths. A 100 W quartz tungsten halogen (QTH) lamp IR source was set up to experimentally measure the fill factor (FF) and the maximum conversion efficiency of the GaSb cells. A spectrally matched narrowband IR spectrum was obtained from the QTH lamp source using a 200 nm bandwidth optical bandpass filter (BPF) with the center wavelength at 1337 nm purchased from PIXELTEQ. The filtered output from the lamp was calibrated using Thorlabs PM100D power meter. The experimental setup for measuring the I-V curve and conversion efficiency of the GaSb cell using the QTH lamp source is shown in Figure 5.1a. The efficiency is computed at different input radiation levels. Figure 5.1b shows the EQE of the GaSb cell (red curve) and the transmittance curve of the bandpass filter (blue curve) as provided by the vendors. Because the filtered thermal emission bandwidth resides near the bandgap region of the EQE curve, there will be minimal thermalization loss within the cells.



Figure 5.1: (a) Experimental setup for measuring the efficiency of the TPV cell. The spectral bandpass filter is not shown in this picture. (b) EQE of the GaSb cell (in red) and transmittance curve of the bandpass filter used to derive the narrowband IR spectrum for characterizing the cells.

5.2 Selective Absorber/Emitter Fabrication

The absorber and emitter were fabricated on the top and bottom surfaces of a polished W substrate purchased from MTI Corporation. The substrate was 25.4 x 25.4 x 0.5 mm in dimensions. For absorber, a 0.64 cm² rectangular area on the top surface was micro-textured to enhance the solar absorption by scanning an IPG Photonics YLP-1/30 nanosecond 1064 nm pulsed laser over the absorber surface using a Galvo. The whole 6.45 cm² area on the bottom surface of the W substrate served as emitter and was composed of a multilayer nanostructure to achieve spectral selectivity. The multilayer structure consists of two layers of Si₃N₄ dielectric and a layer of W sandwiched in between. Based on the simulated analysis of multiple reflectance spectra listed in Table 4.2, case 9 that has two 120 nm layers of Si₃N₄ and a 25 nm layer of W in between was found to provide the combined optimal values of η_{sel} (~71%) and $\varepsilon_{in-band}$ (0.95). For this study, a selective emitter structure defined for case 9 in Table 4.2 was fabricated. The schematic and the real images of the fabricated sample are shown in Figure 5.2.

Prior to the deposition of films, the W surface was cleaned via microwave oxygen plasma cleaning. The deposition rate of the films was calibrated based on ellipsometry measurements. Silicon nitride layers were deposited by plasma-enhanced chemical vapor deposition (PECVD) method in an Oxford Plasmalab System 100 reactor using silane and ammonia gas mixture diluted in argon. The process of mixing high and low frequency powers was employed to minimize silicon nitride film stress and, at the same time, to obtain a higher film density. The substrate temperature during deposition was maintained at 300 °C. The tungsten film was sputtered onto the substrate at room temperature from a high-purity (99.95%) W target at 90W DC power and 0.67Pa Ar gas pressure. α of the micro-textured absorbing surface and the selective emitting surfaces were also experimentally derived from their surface reflectance measurements performed using multiple laser sources and a spectrophotometer device. This process is discussed in detail in the next chapter.



Figure 5.2: (a) Schematic of the planar absorber/emitter structure. Pictures showing (b) the absorber side, where the black region indicates the laser microtextured area, and (c) the emitter side of the W substrate.

5.3 Experimental Setup and Procedure

A complete STPV system was assembled inside a vacuum chamber. Two thin fused silica rods were used to support the W substrate over the GaSb cells (total cell area is 5.92 cm^2) with a spacing of ~1.5 mm. The temperature of the cells and the emitter were monitored using type R thermocouples that were bonded to the cell mount and the substrate using the OB-600 high temperature chemical set cement purchased from OMEGA Corporation. A reflective heat shield was constructed using a gold foil mounted on an aluminum frame using the OB-600 cement. The shield was installed on the absorber side covering only the non-textured area of the W substrate. The spacing between the shield and the substrate was ~2 mm. A 9.5 CFM capacity 2-stage vacuum pump was run to achieve vacuum conditions of ~100 mTorr inside the vacuum chamber. A 300 W continuous wave line-focus laser diode (λ =808 nm) manufactured by Sino Laser Inc. was used to setup a simulated concentrated solar radiation in the lab. The laser is focused on the 0.64 cm²

micro-textured absorbing surface. The incident laser power is varied to achieve multiple steadystate temperatures. During the experiment, the peak power output from the GaSb cells were recorded using a resistive load and multimeters at different operating temperatures. The complete STPV system setup is depicted in Figure 5.3.



Figure 5.3: Experimental setup of the STPV system built for this study. The inset shows the heated absorber/emitter substrate viewed from the top glass window. The absorber-side heat shield was removed in this picture.

In order to achieve the objectives of this study discussed in section 1.3, it is essential to characterize the absorber and emitter surfaces in terms of their optical properties, chemical structures, as well as morphological and physical integrity at high operating temperatures. Various characterization tools and techniques were implemented to measure these properties. The specular reflectance, and hence the spectral absorptivity, of the Si₃N₄/W/Si₃N₄ coated emitter samples was characterized using Agilent's high-performance Varian Cary 5E Spectrophotometer with a spectral range covering from 300-3300 nm. A FEI Quanta 650 scanning electron microscope (SEM) from

ThermoFisher Scientific in conjunction with an attached Energy-Dispersive X-ray Spectroscopy (EDS) was used for analyzing the surface morphology, physical integrity, and elemental composition of the film structure. An M2000 variable angle spectroscopic ellipsometer from J. A. Woollam was utilized for characterizing the thicknesses of the Si₃N₄ and W thin films in the fabricated emitter samples. Similarly, a Zygo NewView 7300 white-light optical profilometer was employed to acquire the surface profile depth measurements of the selective emitter surface. In addition, a setup of a Renishaw inVia confocal Raman microscope with a 405 nm wavelength laser excitation was implemented for analyzing any chemical composition changes in the Si₃N₄/W/Si₃N₄ structure after annealing at high temperatures. A Labsphere RTC-060-SF integrating sphere (IS) was also configured to measure the diffuse reflectivity of the micro-textured absorber at different wavelengths utilizing multiple laser sources (405 nm, 532 nm, 634 nm, 980 nm, 1064 nm, and 1342 nm).

Chapter 6: Results and Discussion

6.1 Characterization of GaSb Cells

The GaSb cells are characterized using the QTH lamp setup described chapter 5. The measured I-V characteristics of one GaSb cell is shown in Figure 6.1a. The FF was computed to be 0.66, which is lower than the manufacturer-reported value of 0.73 in the specification datasheet. The maximum cell conversion efficiency was determined by illuminating the cells with the spectrally matched narrowband input spectrum derived from the QTH lamp source using the 1337-nm BPF. The cell efficiency was measured at varying illumination intensity, which was controlled by the input electrical power to the lamp. The output from the QTH lamp was calibrated using Thorlabs's PM100D power meter. The efficiency was measured for both the unfiltered (broadband) and matched (using the bandpass filter) infrared radiation. The measured cell efficiency for different input illumination levels is shown in Figure 6.1b. The conversion efficiency is significantly better for matched input radiation (shown by red squares in Figure 6.1b) compared to that for broadband incident radiation (shown by blue triangles in Figure 6.1b). This is because there is minimal thermalization and no sub-bandgap loss for the spectrally matched illumination. The maximum conversion efficiency was found to be 26.3%, which is slightly lower than the manufacturerreported value of $\sim 30\%$ for spectrally matched incident radiation.



Figure 6.1: (a) I-V curve of a GaSb cell measured using the QTH lamp source. (b) Comparison of GaSb cell efficiency with a broadband IR source (blue triangles) and a selective narrowband IR emission centered at 1337 nm (red squares).

6.2 Characterization of Absorber/Emitter

The absorptivity of the micro-textured absorbing surface was measured using multiple laser sources (405 nm, 532 nm, 634 nm, 980 nm, 1064 nm, and 1342 nm) and a Labsphere RTC-060-SF IS. The absorptance was found to be nearly uniform (~92%) across the wavelength of 400-1000 nm, and it drops to 87% at 1342 nm. These measurements are shown in Figure 6.2 with magenta triangles along with a second order polynomial fit (magenta curve) that is later used to simulate the reflection loss for solar radiation between 0.4 μ m to 2 μ m. On the other hand, the specular reflectance of the emitter surface was measured using a Varian Cary 5E Spectrophotometer that has a spectral range of 300-3300 nm. The diffuse reflectance for the same surface was also measured at wavelengths 634 nm and 1342 nm using the same IS setup as used for the micro-textured absorber and was found to be negligible (<0.7% of the total reflection) compared to the specular reflectance. Figure 6.2 shows the simulated (red) and measured absorptivity (green) data for the fabricated emitter. The observed difference between the measured and simulated absorption spectra is attributed to inadequate control of the deposited film thickness.

Ellipsometry measurements of the emitter surface revealed that the three films were under deposited by ~8-10% of the aimed thickness. At longer wavelengths, the measured spectra exhibit higher absorptivity values. This is most likely caused by differences in the optical constants of the materials used during fabrication and the values used in the simulation. Despite these differences, the fabricated selective emitter exhibits a good spectral selectivity with a very high thermal emittance right above the bandgap of GaSb TPV cell.



Figure 6.2: Absorptivity of micro-textured W (in magenta triangles) and Si₃N₄/W/Si₃N₄ selective emitter (simulated curve in red and measured values in green). GaSb EQE is shown in black.

6.3 STPV System Results

A 300 W continuous-wave line-focus laser diode (λ =808 nm) was setup to simulate the concentrated solar radiation in the lab. The laser was focused on the 0.64-cm² micro-textured absorbing surface. The STPV system was tested at various operating temperatures by varying the

incident laser power, and the corresponding absorber/emitter temperature and TPV cell output were recorded. The modeled and measured TPV cell output power density, as well as the system efficiency results at different STPV temperatures are shown in Figure 6.3. Both the measured TPV cell output and system efficiency follows the simulation curves closely. A maximum electrical output power density of 1.75 W/cm² was recorded at a temperature of 1670 K. The required incident laser power was 132 W that is equivalent to a solar concentration factor of ~2060 (assuming air mass of 1.5), which is readily achievable with Fresnel lens setup. Note that the simulated output power density and system efficiency plots shown in Figure 6.3 are different than those in Figure 4.13. This is because for a fair comparison with the experimental results, the simulation was rerun using the measured absorptivity spectra of the selective emitter. The modeled system efficiency at 1670K temperature is 10.1%. The experimentally measured system efficiency is 8.6%, when the TPV cell output power density is normalized to the emitting surface area. The difference between the modeled and measured system efficiency is attributable to simplified approximations incorporated at various stages of simulation. One such example is utilizing the measured absorptivity of the emitter at room temperature for simulating thermal emission at higher temperatures. In real, the optical properties of W and Si_3N_4 are temperature dependent [64], [65]. Barnes et al [64] reported a significant increment in the refractive index (n) of W beyond 1.5 µm at 1500K. A TMM simulation showed that the increased 'n' value of W would result in an increased absorptivity at longer wavelengths, thereby suggesting that the actual sub-bandgap loss in our system can be larger than the modeled value. This effect is discussed in more details in chapter 7.



Figure 6.3: (a) Experimental (red crosses) and simulated (black curve for blackbody emitter and blue curve for our selective emitter) TPV cell output power at various absorber/emitter temperatures. (b) Modeled (black curve is for no photon recycling and blue curve is with photon recycling) and experimental (red crosses) STPV system efficiency obtained at various operating temperatures.

6.4 Analysis of STPV System Losses

The individual losses in the system were calculated using the thermodynamic model and the spectral absorptivity of the absorber and emitter surfaces, and are shown in Figure 6.4 for the STPV operating temperature of 1670 K. Each loss is expressed in both watts as well as % of total incident power (in the parenthesis).

Based on the thermodynamic model, the STPV system achieves the steady-state temperature of 1670 K at an incident laser power of 119.8 W. The high sub-bandgap emission causes the greatest system efficiency loss (29%) in our design. η_{sel} must be improved for suppressing the sub-bandgap loss. If the simulated spectral emission of the Si₃N₄/W/Si₃N₄ structure had been achieved for the fabricated sample, the sub-bandgap loss would have reduced by ~50% and the system efficiency would rise above 10%. Additionally, a selective window filter can also be installed in between the emitter and TPV cell for more effective recycling of sub-bandgap photons. This filter needs to be transparent to in-band radiation, and highly reflective at

wavelengths $>\lambda_{BG}$. Previous studies have reported resonance and plasma-interference filter structures based on semiconductors and transparent conducting oxides as potential edge filters for photon recycling in STPV systems [34]–[36]. Alternatively, re-utilization of sub-bandgap photons can also be achieved using metal reflectors at the back interface of TPV cells. Recently, Omair et al. [62] reported 94% sub-bandgap reflectivity achieved by utilizing the photovoltaic band-edge as spectral filter and incorporating a rear gold reflector in a lattice-matched In_{0.53}Ga_{0.47}As TPV cell. A 75% reduction in the sub-bandgap loss in the current system would provide an additional gain of 2.4% in the system efficiency. An alternative approach of harvesting the sub-bandgap photons is by utilizing a multi-junction TPV cell structure. For example, Bendelala et al.[37] proposed a high-efficiency TPV system comprising of a meta-material film based selective emitter coupled to an InAs/GaInAsSb tandem cell, with a theoretical maximum thermal-to-electrical conversion efficiency of ~41% at 1773 K based on simulation.

The combined reflection (P_{ref}) and emission losses ($P_{rad, abs}$) from the absorber side is ~20 % of the input power. The emission from the 4 sides ($P_{rad, side}$), convective (P_{conv}), and conduction (P_{cond}) heat losses is less than 5% of the incident power. The modeled η_e is ~79%. The installation of the Au heat shield is key for achieving such a high η_e . The values of AR and VF in our STPV setup are 10 and 0.91, respectively. Approximately 24 W of thermal power radiated from the emitter is reflected back to the emitter by TPV cells.

The simulated output power density for the GaSb cells at the 1670 K emitter temperature is ~2W/cm², which is ~14% greater than the experimentally measured value. Note that the simulation assumes the TPV cells are maintained at room temperature (300 K). During experiment, the TPV cell temperature was measured to be 321 K that resulted in a ~6% drop in the open-circuit voltage of the GaSb cells. Considering only the in-band portion ($\lambda < \lambda_{BG}$) of the thermal emission
from the emitter, a TPV cell conversion efficiency (η_{TPV}) of 19.5% was achieved at 1670 K. This is lower than $\eta_{TPV}=26\%$ measured during the cell characterization using a narrowband emission from the QTH lamp and filter setup. This significant reduction in η_{PV} is due to increased thermalization loss in the actual experiment. As discussed earlier, the optimal emitter bandwidth for maximal system efficiency is 0.4 µm right above the edge of the bandgap. The bandwidth of the fabricated emitter is much larger (~0.8 µm), thereby causing much larger thermalization loss at shorter wavelengths. Lowering the thermalization loss by reducing the emitter bandwidth can further improve the system efficiency.

Another major loss factor is PV conversion loss (26%) within the GaSb cells that comprises of thermalization loss and losses due to poor FF and EQE values. Significant differences were found between the theoretical (reported in datasheet and literature) and the practical values of FF and EQE for the GaSb cells [41], [44]. η_{STPV} would rise by ~3% if the FF and EQE values had matched the specification. The reflection loss from the absorber surface is 8%. Reducing it to 1% can add 0.6% gain in the system efficiency. Cavity loss is also 8.5% of the total incident power. Therefore, future works should be focused on improving the selectivity of the emitter surface, suppressing the sub-bandgap loss, utilizing more advanced TPV cells with highly reflective metal back surfaces, implementing better thermal management for the cells, and reducing the reflection loss from the absorber surface. The combination of these improvements would lead to an improved system efficiency at 16% or higher.

The monochromatic laser radiation source used to heat up the STPV element in our experiment does not precisely simulate the broadband solar radiation. The reflectance of the micro-textured absorber is greater than 8% for longer wavelengths. The reflection loss computed for the terrestrial solar irradiance (air mass of 1.5) for wavelengths between 0.4-2.0 µm, which covers

95% of the incoming solar radiation, is 9.5%. Owing to this increased reflection loss from the absorbing surface, the overall experimental system efficiency would reduce to 8.4% if tested with a realistic solar simulator, such as a conventional xenon arc light source. In addition, the optical losses in the concentrator setup should be considered when the system operates in real environment.



Figure 6.4: Power flow diagram showing losses at different stages of STPV system operating at T=1670 K.

6.5 Conclusions

STPV is a promising technology to fulfill our future energy needs, given their potential to exceed the SQ limit. A high-efficiency planar STPV system using a micro-textured absorber and a multilayer $Si_3N_4/W/Si_3N_4$ coated selective emitter was fabricated and tested. An absorptivity of 0.92 was measured for the textured absorber for wavelengths below 1 µm. $\varepsilon_{in-band}$ for the selective

emitter was measured nearly 3 times greater than that of a W emitter. Owing to a high VF in our setup, the cavity loss was limited to 8% of the radiated power from the emitter. The excellent thermal management, where the TPV cells were mounted on a water-cooled copper heat sink, prevented excessive heating of the cells during operation. The implementation of the Au heat shield significantly suppressed the thermal emission from the non-active region of the absorber. The performance of the STPV system was evaluated using a 300 W continuous-wave laser as a simulated source for incident radiation. An output power density of 1.75 W/cm² and a system efficiency of 8.6% were recorded at the operating system temperature of 1670K. The required incident solar concentration to achieve this efficiency is 2060X at air mass of 1.5. This experimental efficiency is higher than those of previously reported STPV systems. Various optical and thermal losses occurred at multiple stages of the energy conversion process were quantified. Combining the simulation and experimental results, essential guidelines to further improve the system efficiency were also provided. The experimental STPV results presented in this chapter has been published in the Solar Energy journal [61].

Loss item	Percent of input power	
Reflection off the absorber	8%	
Emission from absorber side	12.9%	
Emission from sides	2.2%	
Convective loss	1.7%	
Conduction loss	1.3%	
VF loss	8.5%	
Sub-bandgap loss	29%	
TPV conversion loss (FF, EQE, thermalization)	26.0%	

Table 6.1: Modeled power losses at each stage of the experimental STPV system operating at T=1670 K.

Chapter 7: Characterization of Surface Absorptivity of the Emitter at High Temperature

Owing to the complexity of STPV systems, a complete thermodynamic simulation of a realistic STPV system is challenging to formulate. Depending upon the complexity of the design, it is sometimes appropriate to incorporate simplified assumptions in the modeling study. One such example is using the measured or modeled spectral absorptivity of the selective emitter at room temperature for estimating the thermal emission at higher temperatures. The same approach was followed in the thermodynamic modeling of the STPV system described in the previous chapters. However, a surface emissivity changes with temperature. Previous studies [64]–[66] have reported that the optical constants of the refractory metals and dielectric thin film layers vary with temperature. The deviation of optical properties at TPV operating temperature may have a direct impact on the surface spectral characteristics of the emitter design. Thus, it is important that the temperature dependency of the material optical constants is considered during the design process and its impact on the emitter performance is characterized and understood well.

This chapter presents the dependence of the surface absorptivity of the $Si_3N_4/W/Si_3N_4$ coated tungsten selective emitter upon temperature ranging from 300 K to 1500 K. Both simulation and experimental methods were used to characterize the surface emissivity as a function of temperature.

7.1 Experimental Setup

For this study, a new selective emitter surface was fabricated using a multilayer structure consisting of two layers of 180 nm Si_3N_4 dielectric and a 40 nm of W layer sandwiched in between, as shown in Figure 7.1a. The fabrication procedure followed the same approach as discussed in

Chapter 5. The sample dimensions are 25.4 x 25.4 x 0.5 mm. A 25.4 x 2 mm rectangular area near an edge of the emitter surface was micro-textured by scanning an IPG Photonics YLP-1/30 nanosecond 1064 nm pulsed laser over the absorber surface using Galvo. The textured area (Figure 7.1b) exhibits high absorption (>90%) at described earlier. Figure 7.1c shows the details of the experimental setup. The selective emitter substrate was supported on two thin fused silica rods and is kept inside a vacuum chamber. The emitter surface is faced up towards the vacuum top quartz window. The reflectivity of the emitter was measured at three wavelengths, namely 633 nm, 1342 nm, and 1550 nm, using laser sources installed outside the vacuum chamber. The laser was incident on the emitter surface through the quartz window at $\sim 30^{\circ}$ angle of incident and the reflected beam was received by a photo detector connected to Thorlabs's PM100D power meter. For each incident beam, three coplanar reflected beams were observed. Two of them were due to reflections from the top and bottom surfaces of the quartz window. The third one was reflected off the emitter surface and was the beam of our interest. The emitter substrate was slightly tilted on one side to isolate the reflected beam of interest from the other two beams. A 300 W continuous-wave linefocus laser diode (λ =808 nm) was set up (not shown in Figure 7.1c) to focus on the micro-textured area of the emitter. The laser-power is gradually increased to achieve multiple high steady-state temperatures. The temperature of the substrate was monitored using a type R thermocouple bonded to the substrate. During the measurement of the reflected beam power for the infrared lasers, a band pass filter (BPF) was also installed in front of the detector to suppress the background noise contributed by the thermal emission from the sample at high temperatures. For each reflectivity measurement, a background noise was first measured by turning the laser off. The background offset is then subtracted from the reflected beam power measured by the power meter. The reflectivity (R) of the emitter is computed as the ratio of the reflected beam power to the incident laser power and is recorded at each temperature. The vacuum condition of ~ 100 mTorr was created inside the chamber using a 9.5 CFM capacity 2-stage vacuum pump.



Figure 7.1: a) Schematic of the $Si_3N_4/W/Si_3N_4$ selective layer. b) Picture of the fabricated selective emitter showing the textured line area where the high-power laser beam is incident for heating. c) Experimental setup for measuring the reflectivity of the $Si_3N_4/W/Si_3N_4$ selective emitter as a function of temperature at multiple wavelengths. The high-power laser for heating is setup orthogonal and is not shown in this figure.

7.2 Optical Modeling

The spectral emissivity of the Si₃N₄/W/Si₃N₄ stack employed in this study was also modeled using TMM as described previously. The required optical constants, refractive index (n) and extinction coefficient (k), for W and Si₃N₄ at room temperature (300 K) were obtained from literature [58], [59]. For Si₃N₄, k is assumed to be zero between 0.5-5.5 μ m, which is the range of simulation used in this study. The spectral reflectance was simulated at 300 K and 1500 K. A number of studies aimed at determining the temperature dependence of n, k, and spectral emissivity of W have been reported in the literature [64], [66], [67]. One experimental study [64] showed that the n value of W significantly increases with temperature at near-infrared wavelengths, and nearly doubles at 2 μ m when the temperature is raised from 300 K to 1500 K. In this study, the n and k values of W

at 1500 K were derived from Barnes' work [64] and were used to simulate the reflectance spectra of the $Si_3N_4/W/Si_3N_4$ stack at 1500 K. Similarly, another experimental study [65] showed that the temperature dependency of the n value and emissivity of Si_3N_4 is minimal below 8 μ m. As such, no change in the n values of Si_3N_4 was incorporated in the TMM simulation at high temperatures.

7.3 **Results and Discussion**

The emissivity of the Si₃N₄/W/Si₃N₄ selective emitter derived from the measurements of the reflected laser beam power at 633 nm, 1342 nm, and 1550 nm as a function of temperature are shown in Figure 7.2. Only specular reflectance is measurable from the current experimental setup. The diffuse reflectance for the same emitter surface was also measured at wavelengths 633 nm and 1342 nm using a Labsphere RTC-060-SF integrating sphere (IS) and was found to be negligible (<0.7% of the total reflection) compared to the specular reflectance [61]. A scanning electron microscopy analysis of the emitter surface revealed that the surface was uniform without any features. At 633 nm, the absorptivity of the Si₃N₄/W/Si₃N₄ emitter was found to have no dependence on temperature between 300-1500 K. For 1342 nm, the absorptivity was found to be nearly stable with a slight increment (~1%) in its value at 1500 K compared to that at room temperature, especially after 800 K. The difference in absorptivity between 300 K and 1500 K is ~3.5%. The increased magnitude of the absorptivity at longer wavelengths can impair the spectral characteristics of the emitter, which is discussed next.



Figure 7.2: Measured absorptivity of the $Si_3N_4/W/Si_3N_4$ selective emitter at (a) 633 nm, (b) 1342 nm, and (c) 1550 nm as a function of temperature.

The radiant flux density emitted from a surface is a function of temperature and can be estimated from the knowledge of its spectral absorptivity and the Planck's blackbody function. Figure 7.3 shows the spectral absorptivity of the $Si_3N_4/W/Si_3N_4$ selective emitter derived from the modeling and experimental measurements. The blue and red curves represent the output of the TMM simulation performed for the emitter temperature of 300 K and 1500 K, respectively. The simulation results show that the change in absorptivity between the two temperatures is minimal for wavelengths less than 1.4 µm. Beyond 1.4 µm, the absorptivity shows a noticeable increment at 1500 K. The spectral absorptivity was also measured between 300-3300 nm at room temperature using the Varian Cary 5E Spectrophotometer and is shown by the green curve in Figure 7.3. There is a good agreement between the measured and simulated spectra at room temperature except at the longer wavelengths, where the spectrophotometer measurements are found noticeably higher. This discrepancy at infrared wavelengths is believed to be caused by differences in the optical constants of the materials used during fabrication and the values used in the simulation. The laserbased absorptivity measurements at 633 nm, 1342 nm, and 1550 nm are also shown with 'x' symbols for temperatures 300 K, ~1000 K, and ~1500 K. The room temperature measurements of absorptivity using lasers exhibit good resemblance with the spectrophotometer data. At 1550 nm,

the simulated absorptivity shows a nearly 4% increment at 1500 K, which is consistent with the data obtained using the 1550-nm laser source.



Figure 7.3: Spectral absorptivity of the $Si_3N_4/W/Si_3N_4$ selective emitter derived from the optical modeling (blue and red curves) and the spectrophotometer measurements (green curve). The laser-based absorptivity measurements performed at 633 nm, 1342 nm, and 1550 nm at three different temperatures are also shown with 'x' marks. The zoomed-in inset highlights the change in measured spectral absorptivity at 1342 nm and 1550 nm. The bandgap wavelength of GaSb is marked with a vertical dashed line.

In order to evaluate the performance of the selective emitter at different temperatures, η_{sel} and $\varepsilon_{in-band}$ are considered as the figures of merit. Table 7.1 summarizes the η_{sel} and $\varepsilon_{in-band}$ values of the Si₃N₄/W/Si₃N₄ emitter computed for different absorptivity curves shown in Figure 7.3. $\varepsilon_{in-band}$ for the measured and modeled absorptivity spectra at room temperature are nearly the same. However, η_{sel} for the measured spectra (using spectrophotometer) is found lower (51.4%) compared to the η_{sel} =64.7% for the modeled spectra at room temperature. This reduction in η_{sel} resulted from the increased absorptivity at longer wavelengths observed for the fabricated sample in the spectrophotometer measurements. The modeled spectra at 1500 K also exhibits a lower η_{sel} value (53.6%) due to the increased absorptivity beyond 1.4 µm. $\varepsilon_{in-band}$ is nearly the same between the 300 K and 1500 K modeled spectra, which is expected as the aggregated absorptivity below λ_{BG} was found to be fairly stable with temperature.

Table 7.1: Spectral selectivity (η_{sel}) and in-band emissivity ($\epsilon_{in-band}$) computed for different absorptivity curves (Fig. 3) of the Si₃N₄/W/Si₃N₄ structure.

Absorptivity of $Si_3N_4/W/Si_3N_4$	η_{sel} (%)	$\boldsymbol{\epsilon}_{\text{in-band}}$
Measured at 300 K	51.4	0.79
Modeled at 300 K	64.7	0.83
Modeled at 1500 K	53.6	0.82

The increased absorptivity beyond λ_{BG} leads to a greater sub-bandgap emission that is not absorbed by the PV cells. In a previous chapter, it has been shown that the sub-bandgap radiation is a primary source for the greatest efficiency loss in TPV systems. Based on the modeled absorptivity of the Si₃N₄/W/Si₃N₄ structure at 1500 K, nearly 46% of the net radiant flux emitted by the emitter is beyond λ_{BG} of the GaSb PV cell. If the modeled absorptivity spectra at room temperature holds true at 1500 K, the sub-bandgap emission would only be ~35% of the total emission. Considering the modeled absorptivity spectra at 1500 K and the partial recycling of the sub-bandgap photons due to the GaSb cell reflectivity, the modeled system efficiency reported in chapter 4 drops by ~11%. Assuming the sub-bandgap loss in the actual system increases by the same proportion, the simulated system efficiency for the experimental setup reduces η_{STPV} from 10.1% to ~9% at 1670 K, which is in a better agreement with the experimentally measured η_{STPV} =8.6%. The noticeable increase in the sub-bandgap emission at higher temperature signifies the importance of considering the temperature dependence of the surface absorptivity in the design of a selective emitter. Effective photon recycling schemes must be incorporated in STPV designs to reflect these unconvertible photons back to the emitter. This topic has attracted great interest in recent years and was already discussed in Chapter 5.

7.4 Conclusions

High-efficiency STPV systems require a selective emitter to match the thermal emission spectrum from the emitter with the characteristic spectral response of the PV cell. A planar Si₃N₄/W/Si₃N₄ coated W selective emitter designed for GaSb-based STPV applications was presented in this chapter. The spectral absorptivity of the selective emitter was measured at room temperature using a spectrophotometer and was found to have good η_{sel} and high $\varepsilon_{in-band}$. The modeled absorptivity based on TMM showed a good agreement with the spectrophotometer data, except at longer wavelengths, where the modeled absorptivity was found lower than the measured values. The dependence of the spectral absorptivity on temperature was investigated using both experimental and optical modeling approaches. For wavelengths less than $1.4 \,\mu m$, the absorptivity was found to have no dependence on temperature. As such, $\varepsilon_{in-band}$ remained stable between 300 K and 1500 K. At longer wavelengths, the absorptivity increased with temperature. At 1.55 µm, the difference in absorptivity between 300 K and 1500 K was measured to be $\sim 3.5\%$, which is also supported by the simulation results. The increased absorptivity at longer wavelengths lowered the η_{sel} value of the Si₃N₄/W/Si₃N₄ selective emitter. At 1500 K, the sub-bandgap emission from the selective emitter was estimated to be nearly 46% of the total emission, which is $\sim 30\%$ greater than that computed using the room temperature absorptivity spectra. The significant reduction in η_{sel} at high temperature thus highlights the need for consideration of temperature dependence of the material optical constants in the design of spectrally selective surfaces. This work has been submitted to the Solar Energy journal for publication [68].

Chapter 8: Thermal Stability Assessment

Another essential factor in STPV system designing is the long-term structural and thermal stability of the absorber/emitter structure. Both W and Si₃N₄ were selected for this study due to their high melting point and near-similar thermal expansivity [69]–[73]. The vacuum conditions during the STPV operation prevent the rapid oxidation of the W surfaces at high temperature. During the acquisition of the experimental data presented in Chapter 6, the system was operated for only a few minutes (less than 5 minutes) at each of the equilibrium temperatures, and no noticeable change in the TPV cell output was recorded during that short record of operation. For practical realization, it is essential to evaluate the system stability for a longer period. In this chapter, scanning electron microscopy, Raman spectroscopy, spectrophotometer and optical profilometer measurements were used to examine any changes in the surface morphology, physical integrity, and the chemical composition of the metal-dielectric films. Similarly, spectrophotometer measurements were also used to characterize any changes in the optical properties of the films after annealing at high temperatures.

8.1 Stability of the micro-textured absorbing surface

The surface morphology of the micro-textured absorbing surface was examined using a FEI Quanta 650 SEM. Figure 8.1 shows the SEM images of the surface before and after annealing at 1600 K for 45 minutes. No noticeable change in the surface morphology was observed, thereby confirming the stability of the microstructures. The absorptivity of the micro-textured surface was measured at different wavelengths using the same setup as described in Chapter 6 using multiple laser sources and a Labsphere RTC-060-SF integrating sphere (IS). After annealing, the absorptance at visible wavelengths (532 nm and 633 nm) was found ~0.90, compared to 0.92 for the same surface prior to annealing. The ~2% decrease in absorptivity can be attributed to a slight

change in the morphology and any formation of oxide layers on the W surface. This will slightly increase the reflection loss from the absorber surface. However, the overall system conversion efficiency will stay essentially the same. Thus, the thermal stability and structural integrity of the textures absorbing surface is less of an issue in our STPV design.



Figure 8.1: SEM images of the micro-textured absorber (a) before and (b) after annealing show no noticeable difference in the surface morphology, thereby confirming the stability of the surface.

8.2 Stability of the metal-dielectric coated emitter

The surface morphology of the Si₃N₄/W/Si₃N₄ coatings as-deposited and after annealing at different temperatures was also examined using SEM. Figure 8.2 shows two SEM images of the surface acquired at different magnifications after annealing the sample to 1670 K for 10 minutes. This is the sample that was used in the experimental STPV system described in Chapter 6. Even for the short duration of annealing, the films were found to develop random cracks, indicating inplane tensile stresses developed at the high temperature [74]–[76]. Over certain cracked areas, the top Si₃N₄ film is found to be peeled off from the W layer (Figure 8.2b). The tensile stress built up in the Si₃N₄ film is attributed to a slight mismatch in the coefficient of thermal expansion (CTE) between the adjacent layers of Si₃N₄ and W. The CTE of W is $4.4x10^{-6}$ K⁻¹ at 300 K, and can rise up to $5.7x4x10^{-6}$ K⁻¹ at 1600 K [69], [72], [77]. Fang et al. [78] measured the CTE of bulk Si₃N₄

as 3.3×10^{-6} K⁻¹ at 300 K, and ~ 6.4×10^{-6} K⁻¹ at 1000 K. Based on the experimentally derived CTE values for Si₃N₄ and W from the literature, an in-plane compressive stress is likely to occur in the Si₃N₄ film at annealing temperatures below ~800 K. A stress reversal occurs at higher annealing temperatures (>800 K), resulting in an in-plane tensile stress that increases with temperature. The occurrence of the random cracks is, therefore, attributed to this in-plane tensile stress developed at the higher annealing temperatures. It is also believed that the compressive stress developed at lower annealing temperatures impaired the adhesion and caused partial delamination between the Si₃N₄ and W films, as shown in Figure 8.2b. A similar thermally-induced structural damage to PECVD Si₃N₄ films at elevated temperatures was also reported by Liu et al. [75].



Figure 8.2: SEM images of the selective emitter surface at different magnifications after 10 minutes of operation at 1670 K.

The cracked areas, where peeling occurred, were also examined with a Zygo NewView 7300 optical profilometer. The surface profile depth measurements of two consecutive craters (left of Figure 8.3) showed that the crack penetrated through the entire thicknesses of the top Si_3N_4 film. The depth of the craters was found to be ~130 nm (right of Figure 8.3), which closely matches with the thickness of the top Si_3N_4 film. This indicates that only the top Si_3N_4 film has peeled off.

An energy-dispersive X-ray spectroscopy analysis performed over the annealed emitter surface also confirmed the presence of a large fraction of W, as shown in Figure 8.4.



Figure 8.3: Zygo NewView 7300 surface profile depth measurements of two consecutive craters (left) of the Si_3N_4 film after the sample treated to 1670 K for 10 minutes. The penetration depth profile (right) showed that the crack penetrated through the entire thicknesses of the top Si_3N_4 film and delaminated from the W film.



50µm

Figure 8.4: (a) SEM image showing the cracks on the Si_3N_4 film. (b) Energy-dispersive X-ray spectroscopy spectra collected from the viewing area shown in (a).

The optical property of the emitter surface was also evaluated before and after the annealing using the Cary 5E spectrophotometer. Figure 8.5 shows the measured absorptivity after annealing at different temperatures and for different intervals. The absorptivity of the selective emitter surface is found to be nearly stable after heating to 1100 K for ~1 h. After operating at 1600 K for 10 minutes, the absorptivity decreased and the peak shifted slightly toward left. The $\varepsilon_{in-band}$ value was found to be lowered to 0.8 from 0.9 at 1100 K. A continuous one hour of operation at 1600 K resulted in a failure of the $Si_3N_4/W/Si_3N_4$ structure (green curve in Figure 8.5). The annealed emitter surface now exhibits visible granular features, as shown in Figure 8.6, with the thin films flaking off at most places. The reflectance of the structure is thus no more specular in nature. This is discussed in more details in the next section.



Figure 8.5: Measured absorptivity of the selective emitter surface after annealing at different temperatures and duration within the STPV system.



Figure 8.6: Visible images of the selective emitter surface (a) before annealing, (b) after gradual annealing treatment to 1600 K in the STPV vacuum chamber for \sim 1 hour.

8.3 Discussion

The reduction in spectral absorptivity of the selective emitter after 10 minutes of operation at 1600 K is a beginning mark of the occurrence of the cracks and the delamination effect in the film as discussed before. Based on TMM simulations, an increased presence of W and a reduction of the Si₃N₄ area on the top surface would result in a lower spectral absorptivity and a right-shifting of the peak absorptivity, similar to the behavior shown in Figure 8.5. This simulation condition is analogous to the peeling off of the top Si₃N₄ film (thereby exposing the underneath W film), as observed over certain areas of the emitter surface.

To understand the failure of the structure after the prolonged heating at 1600 K, a Raman spectroscopy of the annealed sample was performed using a Renishaw inVia Confocal Raman Microscope and a 405 nm laser excitation. The resulting Raman spectra was analyzed using Bio-Rad's KnowItAll Informatics System Software, and the results are shown in Figure 8.7. The black curve is the measured Raman spectra, whereas the red curve is the best-fit spectra from Bio-Rad's database. The measured Raman spectra matches very well with that of tungsten trioxide (WO₃)

with three intense peaks occurring at 806.62, 715.73, and 271.84 cm⁻¹, which correspond to the stretching vibrations of O-W-O and W-O bonds, and the bending vibration of O-W-O, respectively [79], [80]. The occurrence of fractures and the delamination in certain areas of the top Si₃N₄ film exposed the underneath W layer to the air, thereby causing the oxidation of W. The formation of WO₃ is believed to be the primary cause of the structural damage of the multilayer metal-dielectric structure. The melting point of bulk W is 3695 K. However, the melting point for WO₃ drops to ~1740 K [81], [82] (or even lower for nanostructures due to the melting point depression), which is close to the operating temperature of the emitter. The melting of the oxidized W areas further damaged the underlying Si₃N₄ film, thereby degrading the overall structure. Raman spectroscopy performed at multiple locations of the annealed surface show no sign of the crystallization of the amorphous Si₃N₄ film.



Figure 8.7: Measured (black) and fitted (red) Raman spectra of the sample annealed at 1600 K for \sim 1 hour.

Previous studies [75], [83]–[85] have shown that the elastic modulus, hardness, film density, and in-plane stress of Si₃N₄ films deposited using chemical vapor deposition (CVD) are significantly influenced by deposition conditions. An increase in deposition temperature results in

the enhancement of the mass density of the film due to the possible reduction of the elemental composition of hydrogen and excess nitrogen [85]. Similarly, the elastic modulus and hardness were found to increase with the increase in substrate temperature, and with an increase in plasma power and decrease in chamber pressure [84]. Strong correlations between the mechanical properties and film density were also demonstrated [84]. Si₃N₄ films deposited at lower substrate temperature are found to be less stable compared to those deposited at higher temperature [75]. Hughey and Cook [86] demonstrated massive irreversible increases in tensile stress (up to 2 GPa) on thermal cycling of hydrogen-containing PECVD silicon nitride films. Both cracking and delamination of Si₃N₄ films were reported during thermal recycling. It is important to note that most of these studies were conducted in regard to the applications of Si₃N₄ in microelectronics applications and as anti-reflection coatings in systems that operate at relatively low temperatures. Therefore, it is essential to perform similar studies to understand the relation between the various mechanical properties of the film and the PECVD process parameters, which will lead to the formulation of an optimized recipe for depositing high- strength Si₃N₄ films suitable for STPV applications.

As shown in Figure 8.5, the spectral absorptivity of the emitter surface does not show any noticeable change after annealing at 1100 K, thereby implying that the structure of the proposed selective emitter design is stable for operating temperatures below 1100 K. This temperature threshold may not be the most optimal operating range for GaSb-based STPV systems. However, there are other low bandgap TPV cells, such as InGaAsSb (bandgap between 0.29-0.72 eV), for which a selective thermal radiator at 1100 K provides a peak emission near the bandgap wavelength. Therefore, the Si₃N₄/W/Si₃N₄ selective emitter has potential applications in the STPV systems using lower bandgap (<0.5 eV) TPV cells.

The proposed metal-dielectric planar structure for selective emitter is easy to fabricate and offers high spectral selectivity suitable for STPV applications. The PECVD procedure must be refined to improve the structural stability of the planar selective emitter at high temperatures. Denser Si₃N₄ films deposited at higher substrate temperature during the PECVD process exhibited a higher mechanical strength [74], [84]. Furthermore, applicability of other dielectric materials must also be explored for fabricating spectrally selective surfaces. Recently, Shimizu et al [87] illustrated the usage of HfO₂/Mo/HfO₂ nanolayer structures over a Mo substrate for constructing spectrally selective absorber and emitter surfaces. The selective surface was reported to be fairly stable up to 1423 K for ~ 1 hour. Any improvement in the vacuum conditions within the STPV chamber can also prolong the operative lifetime of the emitter by preventing the oxidation phenomena of the refractory metal surface.

8.4 Conclusions

The thermal stability of the micro-textured absorbing surface and the $Si_3N_4/W/Si_3N_4$ coated selective emitter were evaluated using various surface characterizing tools. No noticeable change in the surface morphology of the absorber was found before and after the annealing treatment at temperature of 1600 K. The absorptivity of the absorbing surface reduced from 0.92 to 0.90 at visible wavelengths after annealing. The proposed $Si_3N_4/W/Si_3N_4$ emitter structure was found stable up to the annealing temperature of 1100 K and is, therefore, useful for STPV applications utilizing TPV cells with bandgap less than 0.5 eV. At higher temperatures, the tensile stress builds up due to the differential thermal expansion between the Si_3N_4 and W layers, resulting in the formation of cracks and delamination of the top Si_3N_4 film in some areas. The delamination of the Si_3N_4 film allows oxidation of the exposed W area. The oxidation of W is believed to be the primary cause of the structural damage of the emitter structure during the prolonged operation at 1600 K as the melting point of WO₃ significantly drops to ~1740 K. Further comprehensive studies are required to establish a correlation between the PECVD deposition conditions and the mechanical properties of the Si_3N_4 film so as to come up with an optimal recipe for fabricating thermally stable Si_3N_4 layers suitable for high-temperature applications.

Chapter 9: Conclusions and Future Work

9.1 Conclusions

STPV is a promising technology to fulfill our future energy need, given their potential to exceed the SQ limit. STPV systems are scalable, extremely reliable, and can be used with alternative sources of heat. These features make the STPV technology very appealing for terrestrial and space applications. The main focus of this dissertation was to design, optimize, and fabricate a fully operational high-efficiency planar STPV system and demonstration of high conversion efficiency. A combination of thermodynamic modeling and TMM simulation was used for a detailed-balance analysis of a practical STPV system comprising a planar design using GaSb TPV cells. The study involved comprehensive analysis required for the design and optimization of spectrally selective surfaces that are essential components of high-efficiency STPV systems. Significance of determining the optimal emitter temperature, spectral cut-off wavelength for the absorber, absorber-to-emitter area ratio, and emitter bandwidth for global system optimization was discussed. The relevance of photon recycling on both the absorbing and emitting sides for achieving high thermal extraction and overall system conversion efficiency was investigated.

Utilizing the knowledge gained from the simulation study, a high-efficiency planar STPV system was designed and tested. A micro-textured absorber and a $Si_3N_4/W/Si_3N_4$ coated selective emitter were fabricated on a W substrate. The absorptivity of 0.92 was measured for the micro-textured absorber for wavelengths below 1 μ m. $\epsilon_{in-band}$ for the selective emitter was measured nearly 3 times greater than that of a W emitter. Owing to a high VF in our setup, the cavity loss was limited to 8% of the radiated power from the emitter. The implementation of the Au heat shield significantly suppressed the thermal emission from the non-active region of the absorber. GaSb cells were used for TPV conversion. An excellent thermal management, where the TPV cells

were mounted on a water-cooled copper heat sink, was incorporated to prevent excessive heating of the cells during operation. The performance of the STPV system was evaluated using a 300 W continuous-wave laser as a simulated source for incident radiation. An output power density of 1.75 W/cm² and a system efficiency of 8.6% were recorded at the operating system temperature of 1670K. The required incident solar concentration to achieve this efficiency is 2060X at air mass of 1.5. This experimental efficiency is higher than those of previously reported STPV systems. Various optical and thermal losses occurred at multiple stages of the energy conversion process were quantified. Combining the simulation and experimental results, essential guidelines to further improve the system efficiency were also provided.

This dissertation also studied the dependence of the selective emitter surface spectral absorptivity upon temperature ranging from 300 K to 1500 K. Both simulation and experimental methods were used to characterize the surface absorptivity as a function of temperature. For wavelengths less than 1.4 μ m, the absorptivity was found to have a minimal dependence on temperature. Beyond 1.4 μ m, the absorptivity increases with temperature. At 1.55 μ m, both simulation and experimental data estimated ~4% greater absorptivity at 1500 K than at room temperature. The increased absorptivity at longer wavelengths lowered the spectral conversion efficiency of the selective emitter from 64.7% to 53.6%, thereby resulting in ~ 30% increase in the sub-bandgap radiation loss. This significant increase in the sub-bandgap thermal emission, therefore, highlights the importance of considering the temperature dependency of the material optical constants during the design of a practical selective emitter.

The thermal stability of the micro-textured absorbing surface and the Si₃N₄/W/Si₃N₄ coated selective emitter were also examined using various surface characterizing tools. The absorbing surface did not exhibit any noticeable change in the surface morphology and physical integrity.

However, the absorptivity of the surface was found to be reduced from 0.92 to 0.90 at visible wavelengths after annealing. The Si₃N₄/W/Si₃N₄ selective emitter was found stable up to the annealing temperature of 1100 K. This means the proposed emitter structure is useful for STPV applications utilizing TPV cells with bandgap less than 0.5 eV. At higher annealing temperatures, the tensile stress builds up forming cracks and delamination of the top Si₃N₄ film. The delamination of the Si₃N₄ film allows oxidation of the exposed W area. The melting point of WO₃ is 1740 K, which is close to the operating temperature. A continuous 1-hour operation of the selective emitter at 1600 K resulted in a permanent structural damage. Additional studies are required to derive an improved recipe for depositing thermally stable Si₃N₄ layers suitable for high-temperature applications.

9.2 Future Work

This study provided valuable insights in the optimization of different design parameters for fabricating high-efficiency STPV systems. A system efficiency of 8.6% and output power density of 1.75 W/cm² were experimentally demonstrated. Essential guidelines to further improve the system efficiency were discussed in chapter 6. The high sub-bandgap emission causes the greatest system efficiency loss in the current design. If η_{sel} of the simulated spectral emission of the Si₃N₄/W/Si₃N₄ structure had been achieved for the fabricated sample, the system efficiency would rise above 10%. Re-utilization of sub-bandgap photons can be achieved using TPV cells with metal reflectors at the back interface. A 75% reduction in the sub-bandgap loss in the current system would provide an additional gain of 2.4% in the system efficiency. Second major loss factor is PV conversion loss in the GaSb cells, which resulted from the poor practical values of FF and EQE compared to much higher values reported in the literature. If the reported specification (FF=0.73 and EQE=0.8) were met for the GaSb cells, the system efficiency would rise by an additional 3%.

Narrowing the selective emitter bandwidth to 0.4 μ m can improve η_{TPV} and lower the thermalization loss within the TPV cells. Similarly, the reflection loss from the absorber side was found to be 8%. Reducing it to 1% would further add 0.6% gain in the system efficiency. Therefore, future designs should focus on improving η_{sel} , suppressing the sub-bandgap loss, utilizing more efficient TPV cells, implementing better thermal management for the cells, and reducing the reflection loss from the absorber surface. The combination of these improvements would lead to an improved system efficiency at 16% or higher.

While this dissertation only investigated the use of multilayer metal-dielectric coatings for fabricating the selective emitter, alternative approaches of obtaining spectral selectivity, such as utilizing the photonic crystals [22], [23], [26], 2D surface gratings [21], and periodic pyramidal nanostructures [88], must also be explored for achieving a higher η_{sel} value, and thereby, suppressing the sub-bandgap loss in the system. Future works should also consider utilizing more advanced TPV cells with a built-in back surface reflector for efficient recycling of the low-energy photons.

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Appendices

List of Publications Related to this Work

- 1. E. Pantoja, R. Bhatt, A. Liu, and M. C. Gupta, "Low thermal emissivity surfaces using AgNW thin films," *Nanotechnology*, vol 28, no. 50, 2017.
- R. Bhatt, I. Kravchenko, and Mool Gupta, "High-efficiency solar thermophotovoltaic system using a nanostructure-based selective emitter," *Solar Energy*, vol 197, pp 538-545, 2020, https://doi.org/10.1016/j.solener.2020.01.029.
- 3. R. Bhatt and Mool Gupta, "Development and experimental evaluation of a high-efficiency solar thermophotovoltaic system," submitted to Optics Express.
- 4. R. Bhatt, I. Kravchenko, and Mool Gupta, "Consideration of temperature-dependent absorptivity of selective emitters in thermophotovoltaic systems," submitted to Applied Optics.
- 5. Expected paper based on thermal stability assessment of STPV components.