

Contents lists available at ScienceDirect

Solar Energy Materials and Solar Cells

journal homepage: www.elsevier.com/locate/solmat



Epi-grown broadband reflector for InAs-based thermophotovoltaics

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ABSTRACT

Reflecting sub-bandgap photons is crucial for maximizing the efficiency of thermophotovoltaic devices. However, existing metal-deposited reflectors rely on backside metallization, which cannot be grown epitaxially, necessitating additional processing steps. In this study, we fabricate InAs-based thermophotovoltaic devices featuring a straightforward, epitaxially grown sub-bandgap reflector composed of a single layer of n-doped InAs at a doping concentration of 2.4×10^{19} cm⁻³. This high doping produces long-wavelength metallic-like reflection, and our devices demonstrate high sub-bandgap reflectivity from 3.5 to 17 μ m, achieving up to 93 % reflectivity compared to 30–40 % for designs without the reflector. Using a calibrated optical model, we predict that the sub-bandgap reflectivity of this layer enhances spectral efficiency from 38 % to 79 % under a 600 K normally incident blackbody spectrum. This improvement rivals that of a standard gold back reflector, which achieves a spectral efficiency of 94 %. Additionally, our predictive electrical model, calibrated with fabricated devices, indicates that the reflective layer does not adversely affect the electrical properties of the thermophotovoltaic devices. This sub-bandgap reflector can be integrated into existing InAs-based thermophotovoltaic fabrication processes, eliminating complex substrate removal steps required for traditional gold reflectors.

1. Introduction

A significant amount of waste heat is released into the environment, with approximately 10 % of primary energy lost at temperatures above 600 K [1]. This temperature corresponds to a limiting Carnot efficiency of at least 50 % for a cold sink at room temperature, making it attractive for conversion into electrical power. Solid-state converters are most interesting for waste heat harvesting as they offer superior modularity compared to thermo-mechanical engines [2]. Among solid-state converters, thermophotovoltaics (TPV) and near-field thermophotovoltaics (NFTPV) exhibit some of the highest predicted efficiencies [2]. NFTPV technology involves positioning a heat source within 100 nm of a TPV cell, enabling order of magnitudes higher photon transfer [3]. TPV and NFTPV efficiencies are maximized with small absorber bandgaps to achieve sufficient power output densities, and by reflecting sub-bandgap radiation back to reheat the radiator [4]. InAs is an excellent absorber material for TPV and NFTPV technologies, particularly for 600-1100 K waste heat due to its ideal bandgap of 0.353 eV [5]. According to a detailed balance calculation considering TPV and NFTPV devices with

InAs absorber layers [6], efficiencies can reach 15 % and 46 % for 600 K and 1100 K radiator temperatures, respectively, when the devices are held at room temperature. However, present room-temperature InAs-based devices [5,7–10], have only achieved efficiencies up to 0.5 % for a radiator at 800 K for TPV [5] and 0.015 % for a radiator at 655 K for NFTPV [9] technologies.

One of the main challenges in achieving high efficiencies for NFTPV and TPV systems is mitigating parasitic sub-bandgap photon absorption [2,3,10–12]. At temperatures above 600 K, photons with energy less than InAs's bandgap account for up to 92 % of blackbody irradiance. Minimizing sub-bandgap photon absorption is crucial, as that absorption does not contribute to current production for the devices but increases their internal temperature, negatively impacting performance [7,10], or increasing cooling requirements. For instance, Selvidge et al. [10] reported a 60 K rise in internal temperature, relative to a cold sink, in an InAs-based NFTPV device illuminated by a 733 K radiator. This temperature increase, primarily due to sub-bandgap absorption, resulted in a fourfold reduction in power output.

Better spectral control can be accomplished by tuning the radiator

This article is part of a special issue entitled: Special Issue "TPV Conf. 2024" published in Solar Energy Materials and Solar Cells.

https://doi.org/10.1016/j.solmat.2025.113544

Received 21 November 2024; Received in revised form 1 February 2025; Accepted 21 February 2025 Available online 1 March 2025

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emissivity or incorporating a selective filter between the radiator and the photovoltaic device, both can help to match the spectrum incident on the photovoltaic device to its spectral response [12]. Another spectral control approach replaces the photovoltaic device's substrate with a broadband back reflector, reflecting sub-bandgap photons to reheat the radiator. Promising back reflectors include planar metallic mirrors [3], the airbridge architecture [13,14], and broadband Bragg reflectors [15]. However, these architectures add complexity to the fabrication process and may pose challenges for large-area NFTPV devices [10].

Epitaxially-grown back reflectors can offer simpler device processing. France et al. [16] epitaxially grew a Bragg reflector structure for a III-V solar cell achieving peak reflection of 98 % but with a small bandwidth <100 nm. Instead, we consider a single layer of highly n-doped InAs as a broadband sub-bandgap reflector. This material has over 90 % reflectivity for wavelengths longer than 5 μ m [17–20]. However, there has yet to be a study on integrating such a layer into TPV or NFTPV devices. In this study, we fabricate and characterize TPV devices and use these measurements to calibrate an optoelectronic model. We employ this model to understand the impact of the epi-grown back reflector on device performance and to develop optimal designs.

2. Experimental procedure

2.1. Device fabrication

Two InAs-based devices were grown by molecular beam epitaxy (MBE) on an n-type sulfur-doped InAs (100) substrate, with structures given in Fig. 1. The primary distinction between the structures lies in the exclusion (Design #1, Fig. 1a) and inclusion (Design #2, Fig. 1b) of a highly doped n-InAs sub-bandgap back reflector (BR) layer. The absorber layer of Design #1 was made thinner to minimize growth costs. However, this adjustment does not impact our comparative results between the two designs. The commercial company, Eurofins EAG laboratories, performed secondary ion mass spectrometry (SIMS) on the wafer with Design #2 grown to measure the doping concentrations as a function of the depth, the results are depicted in Fig. 1c and are compared to the values given in Fig. 1b. Metallic contacts were deposited by electron-beam evaporation without thermal annealing. Ni/Ge/ Au layers with thicknesses of 43/30/87 nm were deposited to form back ohmic contacts [21]. Ti/Pt/Au with thicknesses 25/30/50 nm were deposited to form front ohmic contacts [22]. Square devices were defined by mesa etching, where masked samples were submerged into citric acid with hydrogen peroxide at a volumetric ratio of 2:1 for 3.5 h while being mixed with a spinner set to 300 rpm [23]. The citric acid solution consisted of 200 mL of deionized water with 5 g of citric acid powder, pre-stirred for at least 1 h. No antireflection coating was

applied.

2.2. Measurement methods

Two tools were used to measure the calibrated spectral reflectivity of both bare wafers near their centers. First, spectral reflectivity was measured with Bruker's INVENIO Fourier transform infrared (FTIR) instrument coupled with their HYPERION II microscope and their LN-MCT-D316-025 detector, spanning 0.07-0.98 eV. The data were crosscalibrated with spectral reflectivity measured with a calibrated Newport Oriel IQE 200 (QE) tool, spanning 0.78-0.98 eV. The QE tool measured reflectivity for normally incident light, whereas the FTIR tool used an apertured microscope with an approximate maximum incidence angle of 30°. Nevertheless, results from our optical model suggest that light incident at angles between 0° and 30° exhibit similar spectral reflectivity. The spectral reflectivity of the wafers was measured at room temperature (approximately 295 K) and is presented in Fig. 2. Further calibration details for the spectral reflectivity measurements are provided in Supporting Information. Measured and simulated reflectivity presented in this paper assume perpendicularly incident light, as the n-InAs BR layer behaves like a metal which has excellent angle-dependent reflectivity [18].

Current-voltage characteristics of the fabricated square devices were measured using a four-wire configuration with a Keithley 2420 source meter. The cells were vacuum-held on a temperature-controlled, goldplated copper chuck, with the temperature maintained at 298 K by a thermoelectric controller.

2.3. Optoelectronic model

The optoelectronic properties of the devices were simulated within the commercial software Synopsys TCAD Sentaurus (version S-2021.06) assuming the devices were kept at 298 K. The spectral reflectivity of the epi-stacks were simulated with the transfer matrix method while the optical absorption used the model presented in Ref. [3]. The electrical properties were simulated following the two-dimensional model from Ref. [3] based on drift-diffusion theory. The optoelectronic properties of the materials followed that of ref. [3] unless otherwise stated. The Drude model, which is employed to simulate the impact of free carriers on the optical properties of InAs, was adjusted from that in Ref. [3] to account for the overestimation of free carrier absorption [24]. Parameters differing from Ref. [3] include static and high-frequency dielectric constants of 15.15 and 12.25 [25], respectively, a heavy-hole density of states effective mass of 0.6 [26,27], and a heavy-hole conductivity effective mass of 0.46 [27].



Fig. 1. Schematic diagram of the thermophotovoltaic devices (a) without a back reflector (BR) and (b) with a BR. The devices include a front surface field (FSF) layer. P-type doping was achieved with beryllium (Be), while n-type doping was achieved with silicon (Si) for epi-grown layers and sulfur (S) for the substrate. The absorber layer is nominally undoped. (c) Secondary ion mass spectrometry measuring the doping concentration as a function of the depth of the wafer with Design #2. The background colored regions indicate the structure given in (b). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)



Fig. 2. Comparing measured to simulated spectral reflectivity of the wafers with epi-stacks following: (a) Design #1 without a BR and (b) Design #2 with a BR. The measured photon energy range corresponds to a wavelength range of 2–17 μm.

3. Results and discussion

3.1. Measured optical properties

Design #2, which includes a BR layer, demonstrates superior spectral control compared to Design #1, which lacks a BR layer. We measured the spectral reflectivity of the wafers with Design #1 in Fig. 2a and Design #2 in Fig. 2b. As expected, the design with a BR layer has a much higher sub-bandgap reflectivity at photon energies less than about 0.3 eV, reaching up to 93 %, compared to the 30–40 % reflectivity of the design without a BR layer. This flat reflectivity is consistent with low-doped bulk InAs, which has a refractive index of around 3.5. These results suggest that the BR layer is the primary contributor to the increased reflection observed in Design #2.

Our optical model agrees with these reflectivity measurements. To validate the model, we leverage the low absorption of sub-bandgap photons, which generate interference patterns due to the doping-dependent optical properties of the layers. These patterns can be interpreted from spectral reflectivity data. For the model of Design #2, we used the layer thicknesses and doping values shown in Fig. 1b, extracted

from SIMS, resulting in the solid curve in Fig. 2b. For Design #1, we extracted accurate layer thicknesses and doping concentrations by adjusting them to fit the simulated spectral reflectivity with the measurement. These values are provided in Fig. 1a, leading to the solid curve in Fig. 2a. Both simulations agree well with the measurements.

3.2. Predicted optical performance

We analyze the impact of the n-InAs BR layer's doping concentration (within an achievable range, reaching up to 10^{20} cm⁻³ [19]) and thickness on the spectral efficiency, assuming the SIMS measured device structure, and the far-field normally incident 600 K blackbody spectrum. Additionally, we compare their performance to a device with the n-InAs BR layer replaced with semi-infinitely thick gold. Here, the below bandgap spectral efficiency of the mirror ($\eta_{\rm spec}$) is defined as:

$$\eta_{\rm spec} = \frac{P_{\rm bb}(T) - \int_0^{t_{\rm s}} \mathbf{I}_{\rm bb}(T, E)(1 - \mathbf{R}(E))dE}{P_{\rm bb}(T)}$$
(1)

where $P_{bb}(T) = \int_0^\infty I_{bb}(T, E) dE$ is the blackbody power density at tem-



Fig. 3. Optical performance of the Design #2, which includes a back reflector (BR) layer, illuminated by a heat source at a temperature of 600 K. Spectral efficiency (Eq. (1) as a function of (a) the BR layer doping concentration and (b) the BR layer thickness, for a normally incident blackbody spectrum. A BR thickness of 1.11 μ m was used in (a). Bulk gold BR represents a structure where the BR layer in Design #2 is replaced with gold. Spectral absorption distribution within the layers of the thermophotovoltaic device with a 0.7 μ m thick n-InAs BR doped at 10²⁰ cm⁻³, illuminated by (c) a normally incident blackbody spectrum and (d) an undoped silicon radiator with a 0.1 μ m gap between the radiator and TPV device. The black dashed vertical line indicates InAs's bandgap. As expected, near-field irradiance is higher than the blackbody spectrum due to photon tunneling. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

perature *T*, *E*_g is the absorber layer bandgap, I_{bb} is the blackbody spectrum, R is the spectral reflectivity, and *E* is the photon energy. The integral in Eq. (1) calculates the absorbed sub-bandgap irradiance, assuming all photons that enter the substrate are absorbed due to its high absorption coefficient from the (1–2) $\times 10^{18}$ cm⁻³ doping concentration.

Higher n-InAs BR layer doping concentrations enhance spectral efficiency, as shown in Fig. 3a. A device without a BR layer (effectively a doping concentration of about 10^{18} cm⁻³) achieves a spectral efficiency of 38 %, attributed to the reflectivity from the sharp refractive index change at the air-InAs interface on the front surface. Our wafer with Design #2 achieves a spectral efficiency of 63 %. By maximizing the BR doping concentration to 10^{20} cm⁻³, the spectral efficiency can more than double compared to a device without a BR layer and is only $19\%_{relative}$ lower than the spectral efficiency for a gold BR.

At high doping concentrations, the n-InAs BR can be made thinner. Fig. 3b illustrates the impact of BR layer thickness on the spectral efficiency for three doping concentrations: 10^{18} cm⁻³, 2.4×10^{19} cm⁻³, and 10^{20} cm⁻³. The required layer thickness to achieve peak performance decreases as the doping concentration increases. A minimum thickness of 0.7 µm is needed to maximize spectral efficiency at the highest studied doping concentration of 10^{20} cm⁻³, which is 37 % thinner than the minimum thickness required for our fabricated device with a BR doping concentration of 2.4×10^{19} cm⁻³.

Most sub-bandgap photon absorption occurs in the BR layer in farfield and near-field illumination scenarios. We simulated the layer resolved spectral absorption for a TPV device with the optimal n-InAs BR design ($n = 10^{20}$ cm⁻³ and thickness of 0.7 µm), illuminated by a 600 K normally incident blackbody spectrum (far-field, Fig. 3c) and a 600 K undoped silicon radiator at a 0.1 µm radiator-thermophotovoltaic gap (near-field, Fig. 3d). The vertical dashed lines in Fig. 3c,d indicate the bandgap of InAs; only above-bandgap absorption can contribute to current production, which is predicted to be about 11 times larger in our near-field scenario compared to far-field. The near-field above-bandgap absorbed irradiance constitutes 27 % of the total absorption. In comparison, the device with a bulk gold BR shows an above-bandgap absorption of 35 %, and the device without a BR layer exhibits an abovebandgap absorption of 9 % (refer to the Supporting Information for those results).

3.3. Electrical properties

To verify that the electrical properties of Design #2 were not affected by the highly doped BR layer, we characterized the dark current-voltage properties of our fabricated devices at room temperature, calibrated a predictive electrical model, and simulated the impact of the BR layer on the electrical properties. To calibrate the model, two batches of square devices with nominal mesa widths of (700, 600, 500, 400, 300, 250, 200, and 175 μ m) and corresponding nominal top contact widths of (600, 500, 400, 300, 200, 150, 100, and 75 μ m) were fabricated from the wafer with Design #2. A top-view photograph of a batch is shown in the inset of Fig. 4a. The dark current-voltage characteristics of these devices, presented in Fig. 4, were measured on the same day as the mesa etching. Over time (months), the devices' current in reverse bias increased, indicating sidewall deterioration. This sidewall deterioration could be mitigated by replacing the citric acid etchant with a sulfuric acid etchant [18] or by coating the sidewalls with SiO₂ [28].

The measured dark current-voltage properties of the square devices were simulated using a two-dimensional model. In the model, we used the nominal widths of the square devices and chose the width of the top contact pad to match the ratio between the contact and mesa areas of the fabricated devices. Auger coefficients of $C_{\rm p} = 10^{-27}$ cm⁶/s and $C_{\rm n} = 1.1 \times 10^{-26}$ cm⁶/s were used, based on values from literature [29,30]. The front contact resistivity was varied to fit the measured curves, with a value of 1 µΩcm² providing a reasonable fit. This value is within the uncertainty of our measured value from the circular transmission line method (2 ± 1 µΩ cm²). The absorber layer bulk SRH lifetime ($\tau_{\rm srh}$) was varied to fit the measured data, with $\tau_{\rm srh} = 0.19$ µs providing the best fit.

Significant surface recombination is observed at the front metalsemiconductor interface. The current density measured at -0.1 V (J. $_{0.1V}$) is plotted against the ratio between contact and mesa areas of the square devices in Fig. 4a. The $J_{-0.1V}$ increases as the contact pad area approaches the mesa area, indicating perimeter recombination is insignificant, as it would have otherwise resulted in a negative slope [28]. Our model indicates that surface recombination dominates, as shown in Fig. 4b. The recombination mechanisms of two example dark current-voltage curves (the second smallest and second largest devices) are separated into Auger (J_{aug}), radiative (J_{rad}), SRH (J_{SRH}), and surface recombination (J_{surf}) . The dominant surface recombination aligns with the results in Ref. [7], which measured a small shunt resistance for a similar InAs TPV device, causing a dominant diffusion current. In both cases, this parasitic current path is due to an insufficient electron barrier from the front surface field (FSF) layer. This issue could be mitigated by replacing the homojunction FSF with a p-doped larger bandgap material that has a valence band aligned with InAs (ex: InAsSbP) [3]. However, our MBE reactor was not equipped to grow this material.

The highly doped n-InAs BR layer does not impact the device's electrical properties. Our device's $J_{.0.1V}$ nears the measured value of 0.22 A/cm² reported by Lu et al. [7], as shown in Fig. 4a, which had a contact-to-device area ratio of about 0.2 for a similar InAs



Fig. 4. Electrical characterization of the fabricated devices in the dark using the wafer with Design #2. (a) The measured current density at a reverse bias voltage of -0.1 V of square devices (see inset for example of the devices) as a function of the ratio between the metallic top contact area and the mesa area. For comparison, we have included the measured value (orange) of a similar InAs-based TPV device from Ref. [7]. (b) Current density-voltage of the second smallest (left) and second largest (right) square devices, comparing measurement and simulation. The simulated currents include total current *J*, recombination at the metal-semiconductor interface J_{surfs} Auger recombination J_{aug} , radiative recombination J_{rad} , and Shockley-Read-Hall recombination J_{SRH} . The stars connect the data points from (a) to (b). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

thermophotovoltaic device without a BR layer. The similarity in $J_{.0.1V}$ suggests that the BR layer had minimal impact on the material quality of the subsequently grown absorber layer. Additionally, we simulated the dark current-voltage curves of our device with the BR layer but at a doping of 10^{18} cm⁻³ and 10^{20} cm⁻³. In both cases, the current-voltage curves remained unaffected.

4. Conclusion

We fabricated InAs-based thermophotovoltaic devices incorporating a highly doped n-InAs sub-bandgap photon back reflector layer. Optical characterization revealed a $66\%_{relative}$ increase in spectral efficiency for a 600 K blackbody spectrum in devices with a 1.11 µm thick BR layer at a doping concentration of 2.4×10^{19} cm⁻³ compared to those without it. Our calibrated optical model suggests that increasing the BR layer's doping concentration to 10^{20} cm⁻³ reduces the required layer thickness to maximize performance to 0.7 µm-a 36 % reduction-while achieving a spectral efficiency of 79 % for a 600 K blackbody spectrum. The optimized BR layer is expected to have a spectral efficiency that is 19%_{relative} lower than that of bulk gold. Under near-field illumination, the above-bandgap power transfer constitutes 27 % of the total power transfer compared to 9 % for a device without a BR layer. Our calibrated electrical model indicates that the BR layer does not affect the device's electrical properties, provided the material quality remains unaffected by the high doping levels. Preliminary results suggest that the BR layer does not compromise the quality of the subsequently grown absorber laver.

This work demonstrates the potential of an epi-grown n-InAs layer as a back reflector for thermophotovoltaics. This design can be fabricated with a shorter epitaxial growth time by ion implanting the highly doped n-InAs layer into an n-InAs wafer [17] followed by the growth of the thermophotovoltaic structure. Alternatively, the optical performance may be improved by positioning the highly n-doped layer closest to the heat source, reversing the doping profile from pin to nip. In this new configuration, the highly n-doped layer serves as both an FSF layer and a selective spectral filter. Regarding filtering, the layer would reflect sub-bandgap photons before they enter the device, while being transparent to photons near the band-edge due to the Moss-Burstein shift [24]. Further research is required to assess device performance for reversing the doping profile.

CRediT authorship contribution statement

Gavin P. Forcade: Writing - review & editing, Writing - original draft, Visualization, Validation, Software, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. Mathieu de Lafontaine: Writing - review & editing, Supervision, Methodology, Conceptualization. Mathieu Giroux: Writing - review & editing, Software, Resources. Man Chun Tam: Resources, Investigation. Zbig Wasilewski: Writing - review & editing, Resources, Funding acquisition, Conceptualization. Jacob J. Krich: Writing - review & editing, Supervision, Conceptualization. Raphael St-Gelais: Writing review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. Karin Hinzer: Writing - review editing, Supervision, Resources, Funding acquisition. Conceptualization.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used Grammarly and MS Copilot to edit the text. After using this tool/service, the author (s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We thank Robert Hunter for providing a Python package wrapper he built to facilitate interacting with Sentaurus. This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), the New Frontiers in Research Fund (No. NFRFE-2019-00334), the NSERC Discovery (NSERC RGPIN-2024-04784), the NSERC STPG PowerCom (NSERC STPGP-494090-16), the Canadian Foundation for Innovation, and the Ontario Research Fund. Access to Synopsys Sentaurus software was provided by CMC Microsystems.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.solmat.2025.113544.

Data availability

Data will be made available on request.

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