Optimization of GaSb Thermophotovoltaic Diodes with Metallic Photonic Crystal Front-Surface Filters

Abigail S. Licht[1], Corey S. Shemelya[1,2], Dante F. DeMeo[1], Emily S. Carlson[1], Thomas E. Vandervelde[1]

[1]Renewable Energy and Applied Photonics Laboratories, Department of Electrical and Computer Engineering, Tufts University, Medford, MA USA

[2]Department of Electrical and Computer Engineering, University of Kaiserslautern, Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Germany

***Abstract*— A promising technology for waste-heat recovery applications is thermophotovoltaics (TPVs), which use photovoltaic diodes to convert thermal energy into electricity. The most commonly used TPV diode material is gallium antimonide (GaSb). Recently, GaSb TPV diodes were fabricated with front-surface metallic photonic crystal (MPhC) filters to more optimally convert the incident spectrum. This method showed promising initial results, in part due to a shifting of the photogenerated carriers away from the front-surface and into the device. In this paper, we use the Atlas-Silvaco software package to optimize the TPV diode structure for MPhCs. We investigate the addition of an intrinsic region in the device to take advantage of the shifted photogeneration profile from the MPhCs. This design allows for a 10% improvement in internal quantum at the peak MPhC transmission wavelength.**

Keywords—Thermophotovoltaics; GaSb; Photonic Crystals;

I. Introduction

Thermophotovoltaic (TPV) systems capture waste-heat and convert this otherwise unused energy to electrical power. This conversion is achieved via three stages: an emitter, a filter, and a photodiode, as can be seen in Figure 1. A selective emitter is first used to re-shape the incident spectrum from the energy source to one that is better matched for the TPV diode [1]. A filter stage further narrows the spectrum, allowing transmission of only the ideal wavelengths. The filter stage may also reflect below bandgap photons back to the emitter, reducing heat-loads on the photovoltaic diodes and therefore improving the diode conversion efficiency. Finally, the desired radiation is absorbed by the TPV diode, which converts the incident radiation to electrical power.

To advance TPV technology, progress will ultimately depend upon optimization of each stage as well as optimization of the integrated system. In the past decade, however, the majority of TPV research has focused on improving the emitter stage [2-7]. Comparatively less work has been carried out on the filter and diode counterparts [8-15]. In this paper, we first review recent progress in improving the TPV diode stage. We then present our simulation investigation of TPV diodes designed to work with a particular type of filter stage.

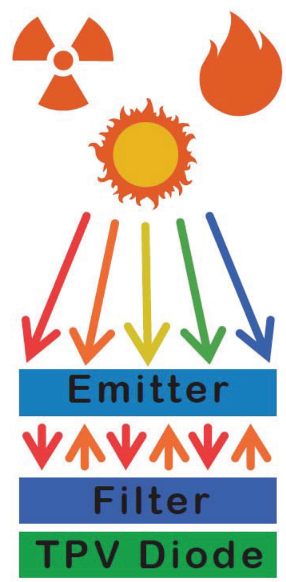

Figure 1: Thermophotovoltaic system: The radiation from a given heat source is absorbed by the emitter, and re-radiated in a band that is closer to the bandgap of the thermpohotovoltaic diode. Additional filtering occurs before the radiation is transmitted to the TPV diode, which converts the incident radition to electrical power through the traditional photovoltaic mechanim.

A. *Advancing the state-of-the-art TPV diode*

A TPV diode typically consists of a thin p-doped top layer and a thicker n-doped absorber/base layer, shown in Figure 2 for reference. At the interface of the doped materials, a depleted space charge region (SCR) forms, with an electric field extending across this region. Charge carriers generated within the SCR, or within a diffusion length of this region, will be accelerated by the electric field, generating a current.

The most common TPV diode material is gallium antimonide (GaSb), which, with a direct bandgap of 0.726eV at room temperature, is optimized for 1400-1600K radiation sources [8]. Commercial GaSb diodes are formed by a singlestep zinc diffusion processes in which zinc is driven into a bulk n-type GaSb substrate, leading to a "p-on-n" configuration with an n-type base [9-10]. Recently, an inverted "n-on-p" configuration was investigated, in which tellurium was diffused into p-type GaSb to form a TPV diode with a p-type base [11]. This configuration is advantageous, as the p-type absorber/base has electron minority carriers, which have much higher mobilities than the hole minority carriers in an n-type base. Tang *et al.* showed that using a p-type absorber allows for improved carrier extraction and, therefore, increased quantum efficiency and power density [11].

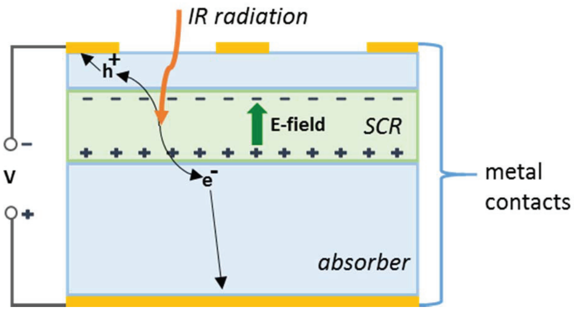

Figure 2: Photovoltaic diode consisting of a top emitter layer and bottom base layer. An electric field is formed over the space charce region (SCR) at the interface of the two regions. Carriers that are generated in the the SCR or diffuse to the SCR are acceleарted due to the electric field, generating a current.

Although more costly than diffusion doped cells, epitaxially-grown diode structures are more efficient. This performance increase is due to a number of reasons –including fewer dislocations which lead to longer carrier lifetimes and higher carrier mobilities [12]. Moreover, epitaxially-defined structures uniquely allow for precise control of the doping profile, enabling sharply-defined junctions which have been shown to lead to higher quantum efficiencies [13]. The epitaxial method allows for incorporation of additional design features, such as incorporating wide-bandgap window layers, which has also proven to directly improve device efficiency [14].

In addition to improvements of the TPV diode, front-surface filtering has been investigated for GaSb diodes through the addition of two-dimensional metallic photonic crystals (MPhCs), Figure 3. These repeating nanoscale structures create photonic bandgaps, providing narrowband confinement of incident photons and, therefore, allowing for transmission of only near-bandgap radiation. The non-infinite depth of the metal/dielectric pattern allows the formation of an evanescent field penetrating into the semiconductor material. The properties of this evanescent field create regions of increased absorption at a greater depth than traditional anti-reflective coatings. By engineering the depth at which the photons are absorbed in the semiconductor, MPhC can mitigate multiple types of recombination mechanisms. MPhCs were first proposed for improving light trapping in TPV diodes in 2012 [16]. Initial work demonstrated an improvement in photogenerated charge carrier profiles by utilizing 2D MPhC as compared to standard diode processing techniques [17].

Given the boost in efficiency for epitaxial structures and promising initial results incorporating MPhCs, this work aims to pursue the marriage of the two ideas. Here we optimize an epitaxially-defined GaSb diode stack for use with a MPhC enhancement. We explore the extent to which this design feature improves the quantum efficiency of the TPV device. This includes exploring the effect of adding an intrinsic region, which would extend the electric field over the shifted photogenerated profile, improving carrier collection and device efficiency.

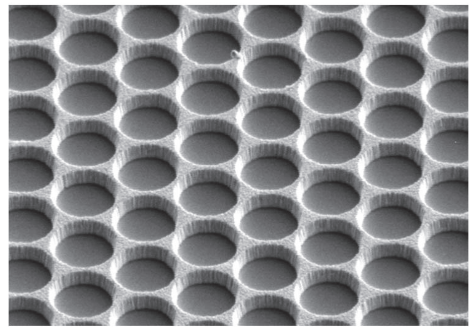

Figure 3: Metallic photonic crystals deposited onto GaSb

II. Simulation and Design

A. Simulation Setup

For bulk GaSb, the majority of the near-bandgap photons ($\lambda \approx 1.7\mu m$) will be absorbed in the top 500-700nm of the material, as can be seen in the plot of the penetration depth of the incident radiation as a function of wavelength, Figure 4. However, when MPhCs are incorporated, the absorption shifts away from the GaSb surface and further into the material, up to a depth of 1.3μm, as determined by finite-difference time domain simulations with the Lumerical simulation software suite, Figure 4. We, therefore, optimize the diode device stack to take advantage of this shifted photogeneration profile.

To simulate the electrical performance of the diode for varying device architectures, we use the Atlas-Silvaco software package. Recombination models enabled included Auger, Shockley-Read-Hall (SRH), and radiative recombination, with parameters taken from reference [19] and listed below in Table I. A modified Caughey-Thomas model was used to determine the mobility as a function of doping [18, 19].

TABLE I. Recombination Models

	Model	***Constant***
Auger	$A(pn^2 - nn_i^2) + A(pn^2 - nn_i^2)$	$A = 5\times 10^{-30}\ cm^6/s$

	Model	*Constant*
SRH	$\frac{pn - n_i^2}{\tau_{SRHn}[p+n_i] + \tau_{SRH}[n + n_i]}$	$\tau_{SRH} = 10\ ns$
Rad	$C(np - n_i^2)$	$C = 8.5 \times 10^{-11}\ cm^3/s$

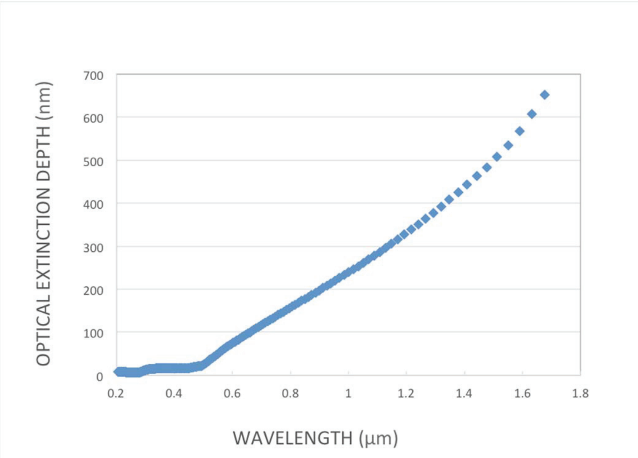

Figure 4: Penetration depth of light in bulk GaSb (here penetration depth is the value at which the intensity of the incident light has decayed to (1/*e*) of the initial value, as calculated from the absorption coefficient).

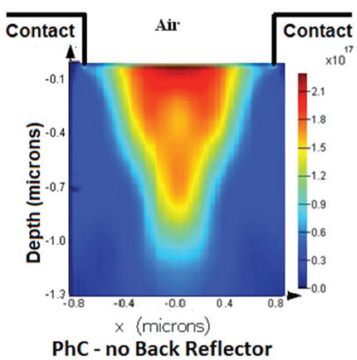

Figure 5: Lumerical FDTD simulation of the absoprtion in GaSb with gold contacts to represent the metallic photonic crystals.

In the simulation, the incident beam is defined as a blackbody with peak wavelength at 1.3µm to correspond to our previous MPhC simulations [20]. This beam, coupled with the effects of the photonic crystals, determine the photogeneration rate. The performance of the device structure is then determined by solving the coupled nonlinear equations for charge transport applied to a 2D mesh grid defining the structure. In the following section, basic design guidelines and constraints will be discussed first and the optimized device structure will be presented subsequently.

B. Design

The top layer for TPV diodes is usually kept thin: ~100-200 nm. This thickness is important in order to maintain high quantum efficiency for shorter wavelength radiation. In the base layer, increasing the thickness increases collection of carriers, but at a cost to the open-circuit voltage. Here we chose a p-type base, which, as discussed previously, leads to improved device performances.

In between the two doped layers, we introduce a non-intentionally doped (n.i.d) intrinsic region, which has not been investigated as of yet for GaSb TPV diodes. The insertion of the intrinsic region extends the SCR, allowing for improved collection of photogenerated carriers. Ideally, the electric field will extend over the entire intrinsic region. In practice, defects are introduced with larger intrinsic regions resulting in charged impurities causing the electric field to fall to zero. Having the intrinsic region extend beyond this value creates “dead space” and is detrimental to the device performance. For GaSb, we find the optimal intrinsic region thickness to be ~1µm.

This structure also includes a highly doped, wide-bandgap back-surface field (BSF) layer. The BSF layer creates a potential barrier for the minority carrier electrons, reflecting them away from the backside and toward the electric field, reducing parasitic rear-surface recombination. For the BSF layer, aluminum antimonide (AlSb) can be used, since the calculated lattice mismatch to GaSb is low (0.65%) and a large potential (barrier height ~3kT) can be formed, as seen in the band structure in Figure 6.

The final proposed structure from top to bottom is as follows: 80nm n-type layer, 1.0µm n.i.d. intrinsic region, 2.8µm p-type GaSb base, and a 100nm AlSb BSF layer, Figure 6. Adding the intrinsic region leads to substantial improvements; more carriers are collected which increases the photocurrent, leading to relative increase in efficiency of 6%. Moreover, at a wavelength of 1.3µm – the peak transmission wavelength for the given MPhC design – the internal quantum efficiency of the diode increases by 10% for this optimized design.

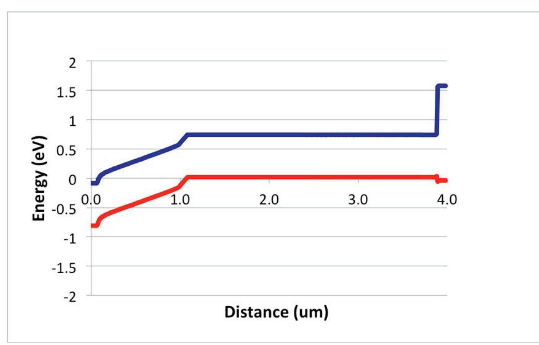

Figure 6: Band alignment: The conduction band is shown in blue and the valence band is shown in red. The device from left to right is an 80nm n-type top layer, 1.0µm n.i.d. intrinsic region, 2.8µm p-doped GaSb base, and a 100nm AlSb BSF layer.

It is noted that anti-reflective coatings have been excluded from this study as they were previously studied with MPhC [20] and found to be less effective. Backside reflectors are of interest and will be included in future work.

III. SUMMARY

In this paper, an inverted n-on-p device architecture for GaSb TPV diodes with front-surface MPhC was proposed. An intrinsic region was added to the n-on-p configuration to take advantage of the shifted photogeneration profile from the MPhCs. This configuration lead to improved collection of photocarriers and therefore an overall relative increase in efficiency of 6%. At the peak MPhC transmission wavelength, the internal quantum efficiency improves by an absolute value of 10%. Given these promising results, GaSb TPV diodes are being fabricated and processed with MPhCs to further explore the effect of this design.

ACKNOWLEDGMENTS

This research was supported by NSF grant EEC1444926. This work was also supported in part by the Intelligence Community Postdoctoral Research Fellowship Program, administered by Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence. We further acknowledge funding from the Office of Naval Research under grant N00014-15-1-2946. Additionally, the authors would like to thank the Alexander von Humboldt Foundation. Finally, this work was performed in part at the Center for Nanoscale Systems (CNS), a member of the National Nanotechnology Infrastructure Network (NNIN), which is supported by the National Science Foundation under NSF Award No. ECS-0335765. CNS is a part of Harvard University.

REFERENCES

[1] N. Pfiester, T. E. Vandervelde, “Selective emitters for thermophotovoltaic applications,” Phys. Status. Solidi. A; 1852-6319, 2016

[2] J. G. Fleming, S. Y. Lin, I. El-Kady, R. Biswas, and K. M. Ho, “All-metallic three dimensional photonic crystals with a larger infrared bandgap,” Nature 417, 52, 2002

[3] J. M. Gee, J. B. Moreno, S. Y. Lin, and J. G. Fleming, “Selective emitters using photonic crystals for thermophotovoltaic energy conversion,” in 29th IEEE Photovoltaic Specialists Conference, New Oreleans, LA, 2002

[4] H. Sai and H. Yugami, Appl. Phys. Lett., “Thermophotovoltaic generation with selective radiators base on tungsten surface gratings,” 85 3399, 2004

[5] S. Y. Lin, J. G. Fleming, and J. B. Moreno, “Three-dimensional photonic-crystal emitter for thermal photovoltaic power generation,” Appl. Phys. Lett. 83(2), 380, 2003

[6] G. B. Farfana, M. F. Sua, M. M. Reda Taha, and I. El-Kady, “High-efficiency photonic crystal narrowband thermal emitters,” Proc. SPIE 7609, 2010

[7] C. Shemelya, D. DeMeo, N. P. Latham, X. Wu, C. Bingham, W. Padilla, T. E. Vandervelde, “Stable high temperature metamaterial emitters for thermophotvoltaic applications,” Applied Physics Letters 104 (20) 201113, 2014

[8] P. S. Dutta, H. L. Bhat, V. Kumar, “The physics and technology of gallium antimonide: An emerging optoelectronic material,” J. Appl. Phys., vol. 81, no. 9, pp. 5821-5870, 1997

[9] A. W. Bett, S. Keser, G. Stollwerck, O. V. Sulima, W. Wettling, GaSb-based (thermo) photovoltaic cells with Zn diffused emitters, in: Photovoltaic Specialists Conference, Washington, DC, 1996

[10] L.M. Fraas, G. R. Girard, J. E. Avery, B.A. Arau, V. S. Sundaram, A. G. Thompson, J. M. Gee, “GaSb booster cells for over 30% effciency solar-stacks”, J. Appl. Phys. 66 3866-3870, 1989

[11] L. Tang, L.M. Fraas, Z. Liu, C. Xu, X. Chen, Performance Improvement of the GaSb Thermophotovoltaic Cells with N-type Emitters, IEEE Transactions on electron devices. Vol. 62m No. 9, pp.2809-2815, 2015

[12] V. M. Andreev, V. P. Khvostikov, V. D. Rumyantesev, S. V. Sorokina, M. Z. Shvartz, “Single-Junction GaSb and Tandem GaSb/InGaAsSb and AlGaAsSb/GaSb Thermophotovoltaic Cells,” Conf. Record of 28th IEEE Photovoltai Spec. Conf. pp. 1265-1268, 2000

[13] N. Quin, Y. Hone, Y. Shu, Q. Lin, “A theoretical discussion on the internal quantum efficiencies of the epitaxial crystal GaSb thin film cells with different p-n junctions,” Solar Energy Materials and Solar Cells, 149, 88-96, 2015

[14] A. W. Bett and O. V. Sulima, “GaSb photovoltaic cells for applications in TPV generators,” Semi. SCi. Tech., 18, S184-S190, 2003

[15] D. DeMeo, C. Shemelya, C. Downs, A. Licht, E.S. Magden, T. Rotter, C. Dhital, S. Wilson, G. Balakrishnan, T. E. Vandervelde, “GaSb Thermophotovoltaic Cells Grown on GaAs Substrate Using the Interfacial Misfit Array Method,” Journal of electronic materials 43 (4), 902, 2014

[16] C. Shemelya and T. E. Vandervelde, “Comparison of Photonic-Crystal-Enhanced Thermophotovtolaic Devices With and Without a Resonant Cavity,” Jouenal of Electronic Materials, Vol. 41, No. 5, 2012

[17] C. Shemelya, D. DeMeo, and T. E. Vandervelde, “Two dimensional metallic photonic crystals for light trapping and anti-reflective coatins in thermophotovoltaic applications,” Appl. Phys. Lettl 104, 021115, 2014

[18] D. M. Caughey and R. E. Thomas, “Carrier mobilities in silicon empirically elated to the doping and field”, Proc IEEE 55 2192, 1967

[19] D. Martin and C. Algora, “Temperature-dependent GaSb material parameters for reliable thermophotovoltaic cell modelling” Semiconductor Science and Technology, 19 p. 1040-1052, 2004

[20] C. M. Shemelya, “Photonics: Photodiodes and metamaterials for Thermophotovoltaics and Photodeection Applications,” Ph.D. dissertation, Electrical and Computer Engineering, Tufts University, Medford, MA 2014