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Study of the effect of 2D metallic photonic crystals on GaSb TPV diode performance

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ABSTRACT

Thermophotovoltaics (TPVs) are a potential technology for waste-heat recovery applications and utilize IR sensitive photovoltaic diodes to convert long wavelength photons ($>800\text{nm}$) into electrical energy. The most common conversion regions utilize Gallium Antimonide (GaSb) as the standard semiconductor system for TPV diodes due to its high internal quantum efficiencies (close to 90%) for infrared radiation ($\sim 1700\text{nm}$). However, parasitic losses prevent high conversion efficiencies from being achieved in the final device. One possible avenue to improve the conversion efficiency of these devices is to incorporate metallic photonic crystals (MPhCs) onto the front surface of the diode. In this work, we study the effect of MPhCs on GaSb TPV diodes. Simulations are presented which characterize a specific MPhC design for use with GaSb. E-field intensity vs. wavelength and depth are investigated as well as the effect of the thickness of the PhC on the interaction time between the e-field and semiconductor. It is shown that the thickness of MPhC has little effect on width of the enhancement band, and the depth the ideal p-i-n junction is between $0.6\mu\text{m}$ and $2.1\mu\text{m}$. Additionally, simulated results demonstrate an increase of E-field/semiconductor interaction time of approximately 40% and 46% for a MPhC thickness of 350nm and 450nm respectively.

Keywords: Thermophotovoltaics, metallic photonic crystals, gallium antimonide

1. INTRODUCTION

Thermophotovoltaics (TPV) is a subset of traditional photovoltaics where light is converted directly into electricity using the photovoltaic effect in semiconductor diodes, however TPV is focused on the infrared (IR) wavelengths. The conversion of IR radiation to electricity has applications in waste-heat harvesting, such as in metal or glass processing facilities, or as a part of nuclear power systems in submarines and space probes. Because of the small bandgap of the TPV diode materials, parasitic losses due to device heating and the absorption of wavelengths below and far above the bandgap are particularly harmful to the device efficiency. This work seeks to investigate the performance and characteristics of a two-dimensional metallic photonic crystal (MPhC) for use in thermophotovoltaic systems to mitigate these losses. Previous work has shown that MPhCs have the potential to improve the conversion efficiency of a TPV diode and by extension the whole of a TPV system¹⁻³. These MPhCs were monolithically integrated into the aperture of gallium antimonide TPV diodes serving as both a front-surface enhancement as well as a topside contact¹. This investigation builds upon the previous work in the field which has demonstrated that photonic crystal enhancements can be used to improve the efficiency of thermophotovoltaic diodes¹. Specifically, this work explores the dependence between the increased e-field interaction time and the thickness of the MPhC in order to achieve optimum TPV diode junction depth and thickness.

Traditional TPV devices are focused on the harvesting of infrared radiation and use various forms of spectral control such as thermal emitters and filters to decouple an energy source from the diode, as depicted in Figure 1. Due to these additional components, TPV can be used in a wider array of application beyond just solar harvesting; one such application being waste heat recovery. The TPV filter stage enables higher system efficiencies by only allowing an efficiently convertible portion of the spectrum to be incident on the diode. This work hopes to further improve upon the TPV filter stage by exploring a MPhC as a combination filter and front-side electrical contact.



Figure 1. Typical components of a TPV system which includes an energy source, an absorber/emitter which absorbs and re-radiates the energy as infrared photons. A filter is then used to further condition the spectrum of light incident on the TPV diode.

Photonic crystals (PhCs) are traditionally periodic arrays of sub-wavelength, dielectric materials that exhibit photonic properties not present in the constituent bulk materials. These structures consist of periodically alternating materials with different refractive indexes to form a photonic bandgap⁴. PhCs have been investigated for use with TPV systems before, however most of this research has been into using them as a selective thermal emitter⁵⁻¹². PhCs have also been used to improve photodetectors and TPV systems through near-field enhancements^{2,6,13-15}. Of specific interest in this previous work is the ability to combine multiple beneficial effects of a metallic structure with the near-field enhancements of a traditional PhC¹.

This near field enhancement is caused by the engineered bandgap of the photonic crystal confining the electric field of incident radiation in the x-y plane for a desired wavelength range⁴. This confinement creates a standing wave within the PhC. The photonic crystals in this work are designed with a specific (non-infinite) thickness which allows leaky-mode propagation in the vertical direction and into the TPV diode region¹³. This narrow-band leaky-mode coupling is expected to increase the potential interaction time with charge carriers in the photodiode and has been shown to increase the short circuit current of the device¹. Additionally, this design can be incorporated into the fabrication process of existing TPV devices and can thus be used as a topside contact grid and in conjunction with an antireflection coating.

However, this technology has not yet been optimized and advances can be made to improve the TPV diode structure for use with a MPhC³ as well as improving the PhC design and fabrication. This work primarily focuses on optimizing the PhC/diode performance for improved total system efficiency.

2. RESULTS AND DISCUSSION

This work focuses on investigating the properties of a front-side MPhC which can be used to optimize the cutoff frequency, electric field depth, and the corresponding ideal junction depth of the TPV diode. Additionally, the dependence of the MPhC thickness on the e-field interaction time was investigated.

Simulations were performed with CST Microwave Studios (2016) using a combination of experimentally obtained (GaSb) and built-in (lossy Au) material parameters. The CST time domain solver uses the finite integration technique (FIT) and was implemented in all the simulations. The same photonic crystal lattice pattern was used from Shemelya et. al.¹. However, simulations were performed for two different thicknesses: the original 450nm, and a new thickness of 350nm, and compared to a control structure of GaSb when applicable. While these were chosen to investigate the thickness of E-field interaction time, it is important to note that these material thicknesses can affect device fabrication. For example, thicker PhC designs can result in a difficult metallization and lift-off process as can be seen in Figure 2, while thinner devices may diminish enhancements.

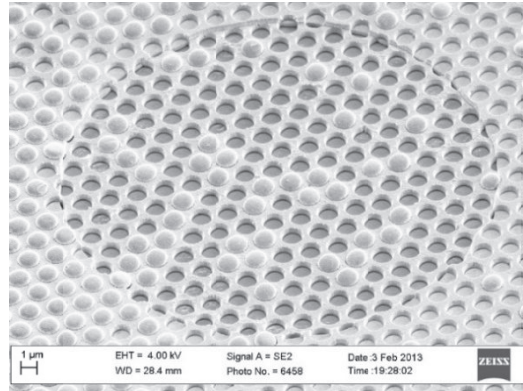


Figure 2: Incomplete liftoff of MPhC holes on TPV diode, reducing MPhC enhancement and increasing "shading" of the TPV diode, decreasing device performance.

2.1 PhC device characterization

The first set of simulations was used to determine the cutoff wavelength of PhC, which was designed to be a few hundred nanometers below the band edge of GaSb. The cutoff frequency of the MPhC, as shown in Figure 4, was $\sim 1.4\mu\text{m}$ which is 310nm below the $1.71\mu\text{m}$ bandgap of GaSb¹⁶. This indicates that the enhancement from the photonic crystal will occur in the spectral range which will be able to be converted by the GaSb diode. It also demonstrates that the MPhC may have a filtering effect on wavelengths longer than $1.5\mu\text{m}$ as compared to a silicon nitride control anti-reflective coating.

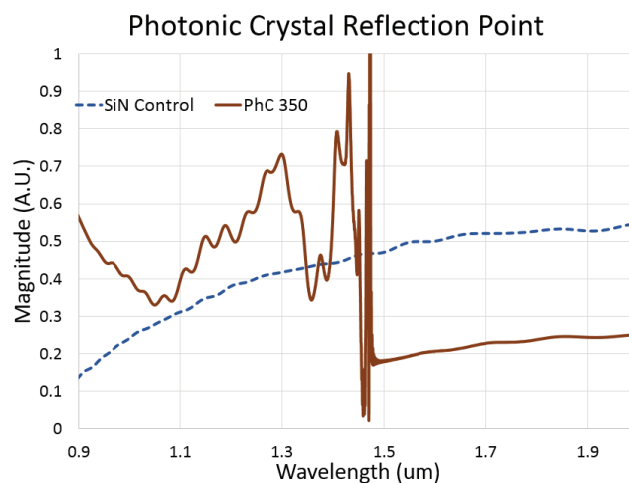


Figure 3. Simulation results of 350nm thick PhC structure showing expected cutoff frequency at approximately $1.4\mu\text{m}$. The SiN control anti-reflective coating provides no filtering effect for low energy photons, while the PhC structure is expected to reduce long wavelength transmission ($>1.4\mu\text{m}$) and reduce phonon creation within the TPV diode.

The depth dependence of the E-field intensity was simulated for both the 350nm and 450nm thick designs and is displayed in Figure 4. Total E-field intensity versus depth is shown on the left, and E-field magnitude versus wavelength on the right. It is important to note that the E-field magnitude between these figures is independent and as such are plotted as A.U. The performance of the two thickness designs is very similar, demonstrating that the e-field profile is dependent more on the lattice spacing and periodicity than the thickness.

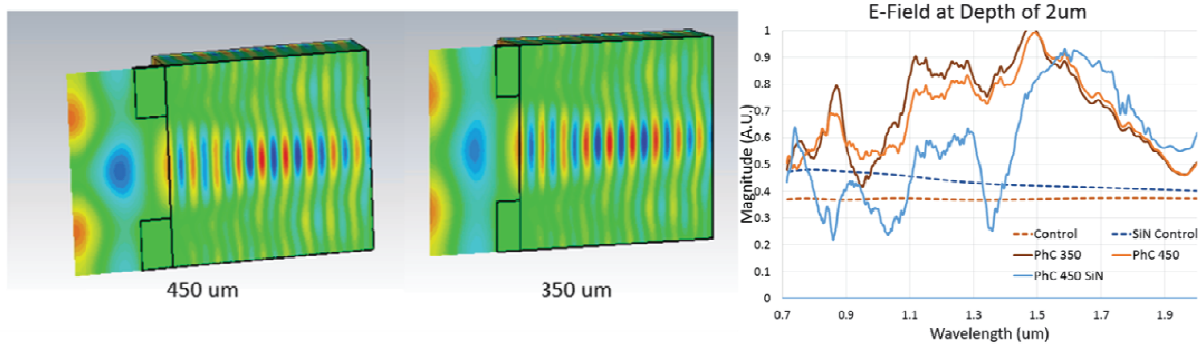


Figure 4. E-field intensity (A.U.) vs depth for PhC thickness of 450nm and 350nm thickness (left) demonstrating the high intensity point located away from the MPhC/semiconductor interface. E-field intensity vs. wavelength at a depth of 2um (right). This shows very similar performance between the two designs, and in the case of the E-field vs. depth a structure thickness of 350nm and 450nm is nearly identical at the wavelengths of interest.

2.2 Optimal Junction Depth

In solid state energy harvesting systems, the physical junction location is of paramount importance, otherwise excitons created through optical excitation will recombine, lowering the efficiency of the system. The junction placement is even more important when implementing a MPhC as the highest E-field intensity is shifted into the semiconductor and no longer follows a traditional exponential decay. To design the proposed structures, the optimal junction depth was simulated and the magnitude of the electric field was observed at multiple wavelengths throughout the GaSb. From these simulations shown in Figure 5, it was determined that the area of maximum enhancement, and therefore ideal junction locations will be between $0.6\mu\text{m}$ and $2\mu\text{m}$ from the MPhC/semiconductor interface.

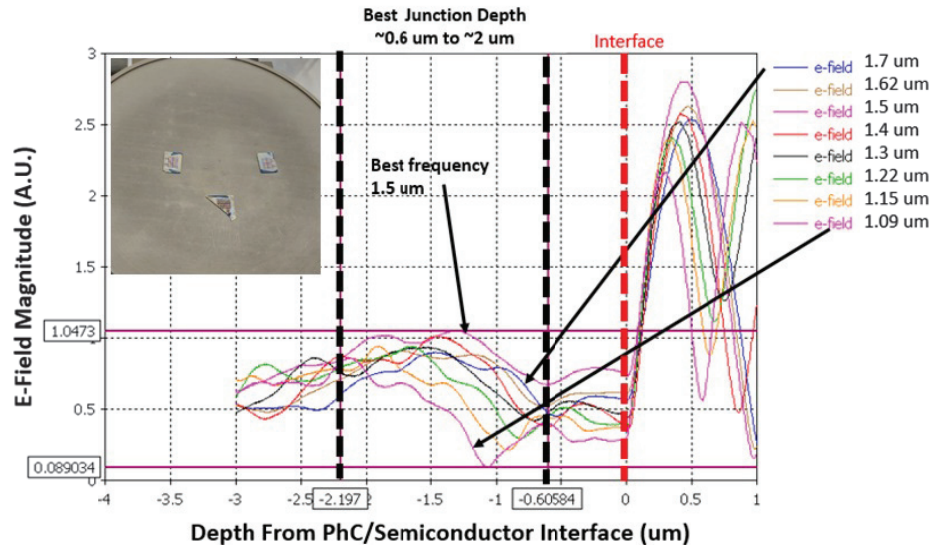


Figure 5. Optimal GaSb junction depth from PhC / semiconductor interface for various wavelengths. Each curve represents a wavelength of interest, and highlighted are the MPhC/semiconductor interface and junction depth. A negative X-value denotes a location in the GaSb, and a positive X-value denotes a location within the MPhC or air. Inset shows the physical diodes based on these simulations in the process of fabrication.

2.3 E-field Interaction Time

In addition to a filtering effect, a non-infinite photonic crystal serves to increase the interaction time between the light and the semiconductor through evanescent coupling. To investigate this effect, a Gaussian pulse was simulated, and the E-field was measured as a function of time within the active area of the semiconductor using CST's time domain solver. The pulse length with an increasing MPhC thickness was measured, as shown in Figure 6, and it was determined that the pulse length increased from 0.013765 picoseconds in the 350nm structure to 0.014467ps in the 450nm structure. When normalized to the time pulse of 0.00987ps with no MPhC present, this demonstrated an increase in interaction time of 39.4% and 46.5% in the 350nm and 450nm PhC, respectively. Therefore, the thicker PhC structure does have a greater the light trapping effect. However, it must be experimentally verified that the 7% increase in carrier interaction time will correspond to a similar increase in diode efficiency.

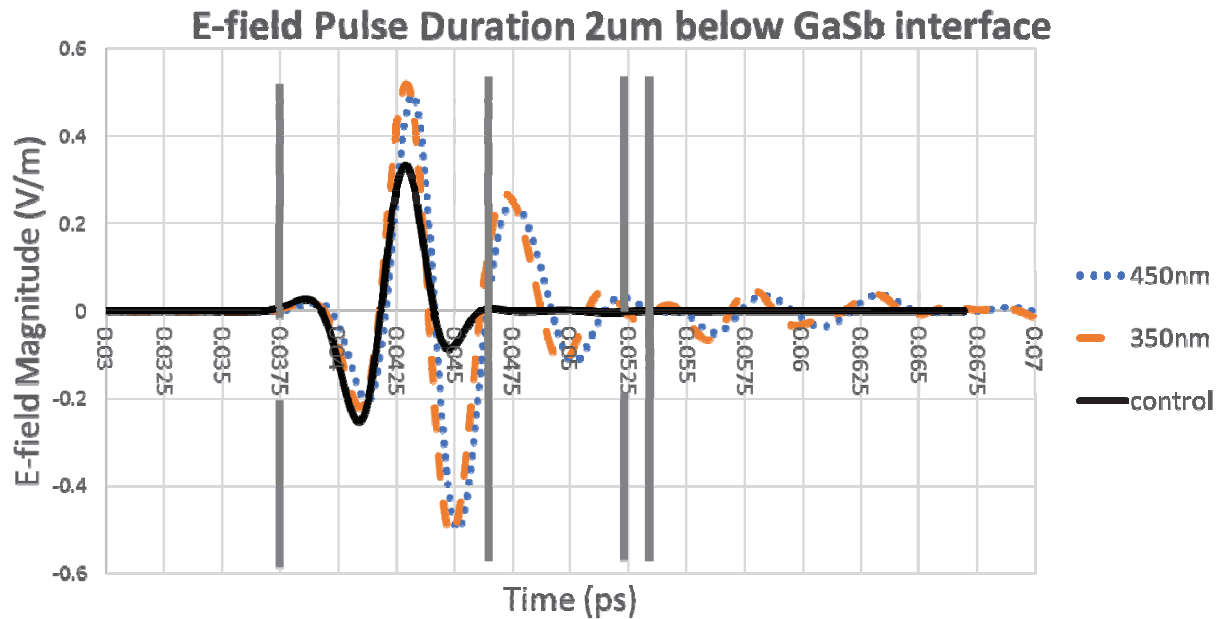


Figure 6. Simulations of E-field interaction time of an electromagnetic pulse incident on a bulk GaSb control (solid black line), 350nm thick PhC design (dashed orange line) and 450nm design (dotted blue line). A conservative estimate was made for the end of the pulse for the PhC designs.

3. CONCLUSIONS

This work serves to investigate and characterize a metallic photonic crystal designed to provide an enhancement to a GaSb thermophotovoltaic diode. It was shown that the MPhC enhancements can be designed for a specific wavelength of interest just below the bandgap of GaSb. The E-field profile as a function of depth and wavelength was found to be similar between different metallization thicknesses. Using these conclusions, it was determined that an optimal junction depth of 0.6 μ m to 2 μ m from the surface of the diode would provide the largest benefit to exciton generation. Additionally, the 350nm PhC design demonstrated a 7% reduction in E-field interaction time when compared to the 450nm design. Although this difference is small, the results indicate that interaction time as well as spectrum within the semiconductor is directly altered by MPhC fabrication tolerances. Further investigation to determine the nature and tolerances of the relationship is warranted. This work provides the design groundwork for future TPV diode structures and metallic photonic crystal designs that optimize interaction time, junction location, and spectral properties.

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