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WITH A BACK SURFACE REFLECTOR

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Monte Carlo Analysis of a Monolithic Interconnected Module with a Back Surface Reflector

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Abstract: Recently, the photon Monte Carlo code, RACER-X, was modified to include wavelength dependent absorption coefficients and indices of refraction. This work was done in an effort to increase the code's capabilities to be more applicable to a wider range of problems. These new features make RACER-X useful for analyzing devices like Monolithic Interconnected Modules (MIMs) which have etched surface features and incorporates a back surface reflector (BSR) for spectral control. A series of calculations were performed on various MIM structures to determine the impact that surface features and component reflectivities have on spectral utilization. The traditional concern of "cavity photonics" is replaced with "intra-cell photonics" in the MIM design. Like the cavity photonic problems previously discussed [1], small changes in optical properties and/or geometry can lead to large changes in spectral utilization. The calculations show that seemingly innocuous surface features (*e.g.*, trenches and grid lines) can significantly reduce the spectral utilization due to the non-normal incident photon flux. Photons that enter the device through a trench edge are refracted onto a trajectory where they will not escape. This leads to a reduction in the number of reflected below bandgap photons that return to the radiator and reduce the spectral utilization. In addition, trenches expose a lateral conduction layer in this particular series of calculations which increase the absorption of above bandgap photons in inactive material.

INTRODUCTION

A photon Monte Carlo code, RACER-X, has been developed and proven to be a useful tool in analyzing and guiding in-cavity thermophotovoltaic (TPV) experiments. RACER-X predictions are routinely within 10% of the measured values for heat absorbed and short circuit current, which is an improvement over the last publication [1]. The code has been modified to model both wavelength dependent refraction and absorption so that it is applicable to a wider range of problems. These new features make RACER-X useful for evaluating designs like Monolithic Interconnected Modules (MIMs) with a back surface reflector (BSR) [2-4].

TPV devices that use a BSR for spectral control must simultaneously balance below bandgap absorption losses with series resistance losses by manipulating the free carriers in each device layer [5]. Hence, the optimal design must consider the combination of photon and electron transport through the multiple layers in the device. The 0.6 eV InGaAs interdigitated MIMs design [6], which is the focus of this study, had been optimized assuming near-normal incidence for photons upon a featureless surface [7]. However, this report demonstrates that optimizing a MIM with a BSR must consider photon angle of incidence effects, detailed surface features, and refraction.

MONTE CARLO MODEL DESCRIPTION

Geometric Description

The analysis in this report is based upon the concept of a 0.6 eV InGaAs interdigitated MIM however, the conclusions are generally applicable to any TPV device that uses a BSR for spectral control. Several TPV diode geometries were constructed and analyzed in an effort to quantify the impact particular geometric features have on spectral utilization and below bandgap reflectivity. MIMs typically require etched trenches on the front surface along with metal contacts. Figure 1 shows the macro-structure of the MIM including the BSR, lateral conduction layer (LCL), and substrate. Notice that the model includes a radiator that is parallel to the top of the TPV surface. Perfectly reflecting boundary conditions were imposed on the four sides of this model to simulate an infinite plate with the MIM structure. Figure 2 shows the details on the surface of the MIM where the photonically important features are the trenches and the grid lines. The back contact trenches in a MIM using an interdigitated grid design are dovetail etched such that they undercut the diode as shown in Figure 2. The isolation trenches are etched as "V-notch" trenches to allow smooth metallization between diodes.

FIGURE 1: Interdigitated MIM macro-structure.

FIGURE 2: Dove-tail back contact trench model.

Several RACER-X models were constructed to isolate the effects of trenches, grids, BSR reflectivity, specularity, diode thickness, and dopant level. This was accomplished by constructing models with and without grids, trenches, etc. and comparing the results. Table 1 provides details of dimensions for individual components used in the computational model.

Optical Properties

Important material properties include wavelength dependent reflectivities and both the real and imaginary parts of the refractive index. Table 2 lists the optical properties of the particular features that were used in the Monte Carlo model. The above bandgap absorption cross-sections were simply modeled with published values of absorption coefficients for binary III-V semiconductors and linear combinations of binary semiconductors for ternary III-V materials [8]. The InGaAs n-type below bandgap absorption coefficients were derived from a Drude model [9], while the InGaAs p-type absorption coefficients were taken from Wilt *et al.* [2]. The degree of specularity is nearly as important as the reflectivity, as is discussed later, so, the percent specularity is also included.

Monte Carlo Results

A series of RACER-X calculations was performed based on a 1750°F radiator and the aforementioned material and geometric description. The radiator was assumed to be a blackbody with a constant 90% emissivity and a diffuse angular emission distribution, (Lambertian). Table 2 shows some selected results from the RACER-X calculations as a function of the geometric and material properties.

The results of most interest are below bandgap reflectively and spectral utilization since they provide useful insight into the performance of the TPV system. Of course, the ideal situation is to have 100% of the below bandgap photons returned to the radiator. Notice that small changes in the below bandgap reflectivity result in large changes to the spectral utilization.

Component	Geometry / Properties
Grid Lines (Gold)	5 μm wide, 4 μm high spaced 100 μm back-to-front contact distance 95% reflective on exposed sides, 0-90% reflective ohmic contact (100% specular)
Back Contact Trench	16 μm wide, 2.1 μm deep dove-tail etch 30° from normal (some models use perpendicular)
Isolation Trench	30 μm wide, 6.25 μm deep v-notch etch 30° from normal (some models use perpendicular)
InP substrate	500 μm thick, $\alpha_{\text{Eg}} = 0 \text{ cm}^{-1}$, $n = 3.6$
N-type Graded Layers $N < 1\text{e}15 \text{ cm}^{-3}$	$t = 2.0 \text{ }\mu\text{m}$, $\alpha_{\text{Eg}} = 0 \text{ cm}^{-1}$, $n = 3.6$
Lateral Conduction Layer N-type 0.6 eV InGaAs $N = 2\text{e}18 \text{ cm}^{-3}$	$t = 0.15 \text{ }\mu\text{m}$, $\alpha_{\text{Eg}} = 580 \text{ cm}^{-1}$, $n = 3.6$
Base N-type 0.6 eV InGaAs $N = 1\text{e}17 \text{ cm}^{-3}$	$t = 2.5 \text{ }\mu\text{m}$, $\alpha_{\text{Eg}} = 0 \text{ cm}^{-1}$, $n = 3.6$
Emitter P-type InGaAs $P = 2\text{e}19 \text{ cm}^{-3}$	$t = 0.1 \text{ }\mu\text{m}$, $\alpha_{\text{Eg}} = 2560 \text{ cm}^{-1}$, $n = 3.6$
Anti-reflection coating	3 layer $\text{MgF}_2/\text{ZnS}/\text{MgF}_2$ - wavelength and angular dependent reflectivity generated with commercially available TFCalc™.
Radiator (Poco-Graphite)	10% reflectivity (100% diffuse)

TABLE 1 - Model Geometry and Optical Properties (t = thickness, α_{Eg} = spectrum weighted below bandgap absorption coefficient, n = real part of index of refraction).

These results demonstrate a number of interesting features for an incident photon flux with a Lambertian distribution, including:

- High impact of either front (grids and trenches) or back surface non-specularly.
- Minimal impact of trench geometry (i.e., perpendicular vs. dove tail / V-notch) (cases 9, 12).
- Minimal impact of ohmic contact reflectivity on spectral utilization (cases 9-11) if there are trenches.

CASE #	Geometric Schematic	BSR Characteristic	Grid Property	Photon Incident Angular Distribution	Spectral Utilization/ Below Bandgap Reflectivity
1	No surface features	100% reflectivity 100% specular	N/A	Perpendicular to surface	77.9% / 95.4 %
2	No surface features	100% reflectivity 100% specular	N/A	Lambertian	77.2% / 95.3%
3	No surface features	98% reflectivity 98% specular	N/A	Lambertian	71.8% / 93.3%
4	Grids only	100% reflectivity 100% specular	95% reflectivity 80% ohmic contact reflectivity	Lambertian	72.1% / 94%
5	Grids only	100% reflectivity 100% specular	95% reflectivity 90% ohmic contact reflectivity	Lambertian	73.4% / 94.5%
6	Perpendicular Trenches Only	100% reflectivity 100% specular	N/A	Lambertian	68.3% / 93.7%
7	Perpendicular Trenches Only	100% reflectivity 100% specular	N/A	Perpendicular to surface	75.2% / 95.6%

CASE #	Geometric Schematic	BSR Characteristic	Grid Property	Photon Incident Angular Distribution	Spectral Utilization/ Below Bandgap Reflectivity
8	Perpendicular Trenches Only	98% reflectivity 98% specular	N/A	Lambertian	55.4% / 88.4%
9	Perpendicular Trenches & Grids	100% reflectivity 100% specular	95% reflectivity 80% ohmic contact reflectivity	Lambertian	60.3% / 90.9%
10	Perpendicular Trenches & Grids	100% reflectivity 100% specular	95% reflectivity 90% ohmic contact reflectivity	Lambertian	60.5% / 91.0%
11	Perpendicular Trenches & Grids	100% reflectivity 100% specular	95% reflectivity 0% ohmic contact reflectivity	Lambertian	59.6% / 90.8%
12	Dove-tail/V-notch Trenches & Grids	100% reflectivity 100% specular	95% reflectivity 80% ohmic contact reflectivity	Lambertian	59.8% / 90.8%
13	Dove-tail/V-notch Trenches & Grids	98% reflectivity 98% specular	95% reflectivity 80% ohmic contact reflectivity	Lambertian	55.0% / 88.5%

TABLE 2 - Racer-X Results with 0.6 eV Interdigitated MIM and a 1750 F Radiator.

ANALYTIC RESULTS

The RACER-X results show that the spectral utilization is surprisingly sensitive to trenches, grids, and BSR characteristics including specularity. As a consistency check of the results, some analytic calculations were performed.

Spectral Utilization Upper Bounds

The key metric for photonic economy is the spectral utilization which is given by,

$$\text{Spectral Utilization} = \frac{\sum_{i=1}^{N_{\text{diodes}}^{\infty}} \int E P_i(E) dE}{\sum_{i=1}^{N_{\text{diodes}}^{\infty}} \int E P_i(E) dE + \sum_{j=1}^{N_{\text{inactive}}^{\infty}} \int E P_j(E) dE} \quad (1)$$

where $P_i(E)dE$ = probability of a photon with energy in dE about E being absorbed in region i . N_{diodes} = number of diodes, and N_{inactive} = number of inactive areas (e.g. busbars, LCL, BSR, etc.).

Thus, the spectral utilization is the above bandgap energy absorbed in the diodes divided by all the energy absorbed in the entire device. Another number that is often cited as a measure of the performance is the below bandgap reflectivity. The spectral utilization is related to the below bandgap reflectivity (R_{bg}), since we can assume that any photons that was not reflected must have been absorbed. Approximately 16% of the total energy of a 1750°F black body radiator is above the 0.6 eV bandgap energy. Assuming that all of the above bandgap energy is absorbed in a device, the spectral utilization at 1750°F is given by,

$$\text{Spectral Utilization} = \frac{0.16 \frac{A_{\text{diode}}}{A_{\text{total}}}}{0.84(1 - R_{bg}) + 0.16} \quad (2)$$

Figure 3 shows a plot of spectral utilization versus below bandgap reflectivity for the idealized case, where there is no inactive area and all the above bandgap energy is absorbed. These calculated spectral utilizations represent an upper bound since they are idealized. Notice that the slope of the curve is steep for high reflectivities. For example, a 95% below bandgap reflectivity results in a spectral utilization of 79%, while a reduction in reflectivity to 92% results in spectral utilization of 70%. As one might expect, it does not take much to change the reflectivity by a few percent.

The upper bound spectral utilizations are consistent with the RACER-X calculations in all cases. Although this adds credence to the RACER-X results, a more detailed analytic calculation is given below.

FIGURE 3: Upper bound spectral utilization versus below bandgap reflectivity.

Analytic Estimation of Spectral Utilization

Another reality check for RACER-X is an analytic estimation of the spectral utilization for the case where there are perpendicular-walled trenches without grids and a 1750°F spectrum of photons incident normal over the entire surface. This problem is simple enough to approximate analytically based on the geometry and the cross sections. Spectrum weighted absorption coefficients were calculated for above and below bandgap energies using the material properties listed in Table 1. These were used to calculate the "survival" probability which is simply the expected attenuation based on the absorption coefficient and material thickness [Table 1]. These survival probabilities are per pass. Given a single layer device mounted to a nonabsorbing insulator and back surface reflector with a single pass survival probability, p , yields a net return of, $(1-p) + (1-p)p$, after two passes.

For this analytic calculation, there are no grid lines and the trench walls are perpendicular. The trenches consume approximately 10% of the surface area so the spectral utilization can be approximated as,

Spectral Utilization =

$$\frac{P_{live} P_{ABG} \bar{E}_{ABG} P_1}{P_{live} P_{ABG} \bar{E}_{ABG} P_1 + P_{dead} P_{ABG} \bar{E}_{ABG} P_2 + P_{live} P_{BBG} \bar{E}_{BBG} P_3 + P_{dead} P_{BBG} \bar{E}_{BBG} P_4} \quad (3)$$

where, P_{live} = the probability of a photon hitting "live" material (diode), P_{dead} = the probability of a photon hitting "dead" material (trench), P_{ABG} = the probability of a photon being born above the bandgap energy, P_{BBG} = the probability of a photon being born below the bandgap energy, $\bar{E}_{ABG}$ = the average energy of an above bandgap photon (at birth), $\bar{E}_{BBG}$ = the average energy of a below bandgap photon (at birth), P_1 = the net probability that an above bandgap photon that hits the diode is absorbed in live material, P_2 = the net probability that an above bandgap photon that hits the trench is absorbed in dead material, P_3 = the net probability that a below bandgap photon that hits the diode is absorbed in live material, and P_4 = the net probability that an above bandgap photon that hits the trench is absorbed in dead material.

The net absorption probabilities require knowledge of the survival probability, and two passes are always assumed. Any photon that hits the diode has the opportunity to go through the p-layer, the n-layer, the lateral conduction layer, and then reverse to go back through the layers. This leads to some complicated net absorption probabilities as given by,

$$\begin{aligned} P_1 = & (1 - P_P^{ABG}) + P_P^{ABG} (1 - P_N^{ABG}) + P_P^{ABG} P_N^{ABG} (1 - P_{lcl}^{ABG}) \\ & + P_P^{ABG} P_N^{ABG} P_{lcl}^{ABG} (1 - P_{lcl}^{ABG}) + P_P^{ABG} P_N^{ABG} P_{lcl}^{ABG} P_{lcl}^{ABG} (1 - P_N^{ABG}) \\ & + P_P^{ABG} P_N^{ABG} P_{lcl}^{ABG} P_{lcl}^{ABG} P_N^{ABG} (1 - P_P^{ABG}) \end{aligned} \quad (4)$$

Other probabilities are derived in similar fashion, resulting in a set of probabilities listed in Table 3. Given these probabilities, the spectral utilization is calculated to be 74.8% with trenches. Eliminating the "trench" terms in the spectral utilization equation (terms 2 and 4 in the denominator of Eqn. 3) the spectral utilization is 77.1%. These numbers are in good agreement with the RACER-X calculations of 75.2% and 77.9%, respectively. The slight inconsistencies could be due to the anti-reflective coating that is modeled in the Monte Carlo code and not in the analytic calculation. Furthermore, the below bandgap reflectivity can be easily calculated as an area weighted fraction,

$$R_{BBG} = 0.9(1 - P_3) + 0.1(1 - P_4) = 94.9\% \quad (5)$$

which again is in good agreement with the RACER-X value of 95.3%.

Variable	Value	Variable	Value
P_1	98.6%	P_P^{ABG}	91.0%
P_2	24.83%	P_P^{BBG}	97.5%
P_3	5.50%	P_N^{ABG}	14.9%
P_4	1.792%	P_N^{BBG}	100%
P_{ABG}	6%	P_{live}	90%
P_{BBG}	94%	P_{dead}	10%
E_{ABG}/E_{BBG}	3.22		

TABLE 3 - Probabilities utilized in analytic calculation

The RACER-X calculations compare well to the analytic calculations for simple geometries. Analytic calculations for non-normal incident photons and/or more complex geometries are nearly impossible given the added complexity of refraction and light trapping.

ANALYSIS OF RESULTS

Refraction and Light Trapping

Refraction in a device with a back surface reflector becomes an important issue because some photons can get sent off at an angle where they get internally reflected and cannot escape. This is analogous to light trapping in numerous optoelectronic devices: solar cells [10], light emitting diodes [11], and quantum well infrared photo-detectors (QWIPs) [12]. The refracted angle, θ_2 (with respect to the surface normal), can be calculated based on the incident angle, θ_1 , and the index of refraction in both materials, N_1 and N_2 , respectively using Snell's law,

$$N_1 \sin \theta_1 = N_2 \sin \theta_2. \quad (6)$$

The refracted angle can never be greater than 90° from the normal, which poses a problem when traveling from high index to low index. In this case, there are a range of incident angles that result in total internal reflection since refraction beyond 90° is impossible. The typical index of refraction for these TPV materials is 3.6, while that of

air is 1.0. Photons that travel from the MIM device towards an air (vacuum) interface must hit the surface at an angle less than 16° from the surface normal to be refracted, otherwise they are reflected.

Non-specular reflection from the BSR reduces the overall reflectivity of a device because once a photon has an angle greater than 16° from the normal, it is internally reflected. Based on a Lambertian distribution for diffuse scattering, the probability of scattering within 16° of the surface normal is given by,

$$P_{0-16} = \int_0^{16} \sin\theta \cos\theta d\theta = 0.038. \quad (7)$$

Thus, only 3.8% of the diffusely scattered photons are within 16° of the surface normal.

Another way a photon can become internally reflected is by entering the MIM via a trench edge. Figure 4 shows a schematic of the incident and refracted ray when it hits a trench. Trenches act as a black absorber for photons since effectively all that enter, get absorbed.

FIGURE 4 - Refraction through a trench

The calculations show that the trenches and grids have a large impact on the spectral utilization. Trenches reduce the spectral utilization in two ways. First, photons entering a trench edge have little hope of escaping due to refraction and subsequent internal reflection. Second, above bandgap photons that enter via the trench bottom are much more likely to be absorbed in the LCL than photons entering the diode. Along with the trench refraction issues, the BSR specularly and reflectivity are important. A non-specular scattering event from the BSR almost always guarantees a trapped photon which, again, greatly affects the spectral utilization.

Quantifying the Effect of Surface Features

RACER-X was used to determine the sensitivities to the various surface features and the results are summarized in Table 4. Trenches have the greatest negative impact on the spectral utilization. The effect of these trenches is magnified when coupled with grid lines. In the interdigitated MIM design that was analyzed, the grids in the back contact trench are taller than the trench itself, which tends to scatter more photons into the walls of the trench [Fig. 5]. Clearly, reducing the trench width will have a positive impact on the spectral utilization without adversely affecting the electrical properties of the device.

The calculations suggest that even with no trenches, the spectral utilization will be approximately 65% for a MIM with a 98% reflective, 98% specular BSR, and grid lines. Thus ensuring that a 100% specular back surface is critical.

MIM/BSR Feature (the starting point for all differences is a featureless MIMs with a perfect BSR)	% Reduction on Spectral Utilization	% Reduction on Below Bandgap Reflectivity
Adding perpendicular trenches	-11.5%	-1.7%
Adding Dove-tail and V-notch trenches	-12.4%	-2.0%
Adding grids	-4.9%	-1.0%
Adding grids and Dove-tail/V-notch trenches	-22.5%	-4.8%
Reducing the BSR specularity to 98% (still 100% reflective)	-7.0%	-2.2%
Adding grids and Dove-tail/V-notch trenches and reducing the BSR reflectivity and specu- larity to 98%	-28.7%	-7.2%

TABLE 4: Racer-X predicted sensitivities for Interdigitated MIM device with properties listed in Table I.

CONCLUSIONS

A detailed photonic analysis is necessary when optimizing a TPV device that utilizes a back surface reflector for spectral control, especially when dealing with a non-normally incident photon flux which is expected in prototypical environments. Surface features like trenches that occupy a small fraction of the surface area can have an enormous impact on the device efficiency.

In addition, spectral characterization of fully fabricated MIMs is required which include multiple angle of incidence reflection measurements and total power absorption measurements. As this analysis demonstrated, measurement of near-normal incidence on unprocessed MIM structures, over-estimates spectral utilization in a cavity environment. These measurements are difficult to perform accurately due to the non-specular nature of a processed MIM and the high accuracy required for values of reflection greater than 90%. Thus, in-cavity heat absorption measurements may prove to be a more useful measure of spectral utilization [1].

This analysis has also highlighted some improvements that may be made to existing MIM designs that will help mitigate the reduction in spectral utilization of a fully processed MIM, these include:

- Minimize trench area. This will require tighter lithographic tolerance to prevent diode shorts.
- Plating of metallization to mushroom over trenches.
- Increase base thickness to increase above bandgap absorption in the action diode area and not in the lateral conduction layer. This will occur at the expense of a decreased open circuit voltage.
- Increase the bandgap of the lateral conduction layer to prevent absorption of above bandgap photons.
- Lower the bandgap of the active layers or increase radiator temperature. This will decrease the sensitivity of the spectral utilization by decreasing the fraction of below bandgap photons.
- Ensure a highly specular back surface reflector. A 2% reduction in specularity reduced spectral utilization by 7%.
- Utilize a front surface interference filter to reflect near bandedge (2-5 micron) below-bandgap photons. This must be balanced with the useful transmission and absorption of above bandgap light.

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