TPXSIM: A MODELING TOOL FOR HIGH EFFICIENCY THERMOPHOTOVOLTAIC SYSTEMS

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Abstract

Thermophotovoltaic (TPV) devices convert heat to electricity using thermal radiation to illuminate a photo-voltaic (PV) diode. Typically, this radiation is generated by a blackbody-like emitter. Such an emission spectrum includes a broad range of wavelengths, but only higher energy photons can be converted by the PV diode, which severely limits efficiencies. Thus, introducing a selective emitter and filter to recycle unwanted photons could potentially greatly enhance performance. In this work, we consider a rare earth-doped selective emitter structure to increase the number of photons emitted above the bandgap of the photovoltaic (PV) cell, while minimizing the total power emitted below the bandgap. A chirped dielectric stack is introduced on top to limit emitted wave-lengths, while a broadband dielectric mirror on the bottom ensures unidirectional emission. We developed a GUI-based tool to precisely calculate the emittance spectrum and efficiency for this design as various parameters, such as the number of dielectric bilayers and PV cell bandgap. The tool is hosted and run through nanoHUB.org - an open-access science gateway for cloud-based simulation tools and resources in nanoscale science and technology. Through simulations of chirped dielectric stack structures and coatings on a rare-earth ceramic substrate, it is found that an efficiency of 33.89% is achievable, for a filter bandgap of 0.37 eV and PV bandgap of 0.75 eV. The research thus demonstrates the potential for unprecedented efficiencies of TPV cells. These predictions will be used to experimentally fabricate and characterize these structures.

1. Introduction

The estimated US energy supply was 97 quads in the year 2013 according to the US Department of Energy. But 61% of this energy was simply rejected as waste heat. These losses, also known as parasitic losses, are partly due to high energy losses in our everyday used electrical appliances like electric ovens and light bulbs. In most incandescent light bulbs, the efficiency of generating light is less than 5% because a significant amount is lost as infrared radiation that only heats up its environment. Similarly, in thermophotovoltaics, the average efficiencies do not approach theoretical limits, thanks to the excessive parasitic losses in the electricity generation process. This research aims to enhance the efficiencies of TPV cells by greatly reducing the amount of parasitic losses.

Thermophotovoltaic cells convert heat energy to electrical output. A typical TPV cell consists of an emitter to emit photons and a photovoltaic cell to generate electricity from incoming photons.

A blackbody or greybody is generally used as the emitter; however, this choice severely limits efficiencies, since the emission spectrum spans a wide wavelength range, including unwanted long wavelengths with insufficient energy to overcome the bandgap in the photovoltaic cell. Thus, a filter is sometimes added between the emitter and the PV cell to reflect low energy photons and consequently recycle them. In this study we propose a selective emitter that not only achieves 100% emittance near the cavity resonant frequency of a rare earth based material, but also cuts down on long wavelength photons and the need for photon recycling.

Thermophotovoltaics are a good source of electricity because they can input energy from a wide range of sources including the sun. Also they are used because they are easily portable which makes them suitable for remote site electricity generation.

In research by Bermel *et al.* [1], the efficiency of a TPV system was enhanced to 26% by introducing a rugate filter design which facilitated photon recycling of lower energy photons. In other work by Celanovic *et al.* [2], a vertical enhanced cavity resonant emitter (VERTE) was proposed. VERTE allows 100% emittance peaks around the cavity resonant wavelength. It uses the concept of Q-matching in which the losses in the cavity equal the losses in the material surrounding the cavity thus resulting in 100% absorption or alternatively 100% emission. In another study conducted by Chubb *et al.* [3], it was shown that rare earth materials can emit photons in several narrow bands. For this reason, we use Erbium Aluminum Garnet as the rare earth material capable of producing photon emission in near infrared region of the electromagnetic spectrum.

2. Methodology

The model proposed for the emitter is a rare-earth based material ErAG cavity with dielectric mirrors on both sides. Dielectric mirrors are alternating stacks of lower and higher order refractive indices. Chirping is when the period of the alternating layers of the dielectric mirror varies according to a function, say exponentially, logarithmically or linearly.

The dielectric mirror at the bottom acts as an almost perfect mirror efficient enough to reflect 99.99 % radiation. The top dielectric mirror is chirped. The structure proposed allows 100 % emittance. The top dielectric layer helps in Q-matching by making the amount of losses inside the ErAG cavity equal to the losses in the top layer. The perfect reflection from the bottom layer and the chirping in the top layer help trap radiation inside the cavity, resulting in 100 % absorption inside the cavity at selected resonant wavelengths. Kirchhoff's law of thermal radiation dictates that 100% absorption results in a 100% emission near the cavity resonant wavelength. Also because of our preference of ErAG, the resonant wavelength is near infrared region which lies in the PV bandgap, thus improving efficiencies.

2.1 Simulation Approach

Stanford Stratified Structure Solver (S4) is a tool developed by Stanford to solve linear Maxwell's equations in layered periodic structures [7]. S4sim is an extension to S4 developed by Purdue University as an analysis of optical propagation in the generalized 3D structure much more quickly than many other alternatives. It inputs a control file in LUA programming language and outputs an absorption/emittance spectrum.

The emittance values calculated for the wide range of wavelengths are then used according to the following formula to compute the photovoltaic current density and the dark current density.

$$J(V) = \int_0^\infty d\lambda \left[\frac{2qc}{\lambda^4}\frac{\varepsilon(\lambda)\mathrm{EQE}(\lambda)}{\exp(hc/\lambda kT)-1}\right] - \left[\frac{q(n^2+1)E_{\mathrm{g}}^2 kT_{\mathrm{d}}}{4\pi^2\hbar^3c^2}e^{-E_{\mathrm{g}}/mkT_{\mathrm{d}}}+J_{\mathrm{nr}}\right]\left(e^{qV/mkT_{\mathrm{d}}}-1\right)$$

Dark current flows in the photovoltaic cell even without the cell in operation. Photovoltaic current, however is produced when photons emitted fall on the photovoltaic cell transferring energy to electrons that jump from their valence band to conduction band. The fill factor (FF) is the ratio of the max power to the product of open circuit voltage and short circuit current. The short-circuit current J_{sc} and the open-circuit voltage V_{oc} are the maximum current and voltage respectively from a solar cell. As FF is a measure of the "squareness" of the IV curve, a solar cell with a higher voltage has a larger possible FF since the "rounded" portion of the IV curve takes up less area (6). The formula for FF is given as:

$$FF = \frac{J_m V_m}{J_{sc} V_{oc}} \ ,$$

where J_m and V_m are the current and voltage at the maximum power point, respectively. These are determined by taking the derivative of the power and setting it to zero to find the maximum value, i.e., with $\frac{d}{dV}(JV) = 0$, then solving for V_m, and finally substituting into the current-voltage relation to obtain J_m.

The power conversion efficiency is then calculated according to the following formula:

$$\eta = \frac{FF \cdot J_{sc} \cdot V_{oc}}{P_{in} - P_{reabs}}$$

Efficiencies were mathematically calculated to be around 34% and simulations were carried out to verify analytical results. Two other useful terms used to determine the quality of the TPV system are radiation efficiency and Emissivity.

Radiation Efficiency $\eta_{rad}(T)$is the ratio between the useful emitted power above the bandgap that can be converted into electricity to the total radiated power at a given temperature T. It is calculated using the following formula.

$$\eta_{rad}(T) = \frac{\int_0^{\lambda_g} d\lambda\, \epsilon(\lambda) I_{BB}(\lambda, T)}{\int_0^{\infty} d\lambda\, \epsilon(\lambda) I_{BB}(\lambda, T)} \ ,$$

where $I_{BB}(\lambda, T)$ is the blackbody emission spectrum at a given temperature T. The emissivity is the ratio of the power emitted by the selective emitter to the power radiated by a blackbody at the same temperature, calculated as:

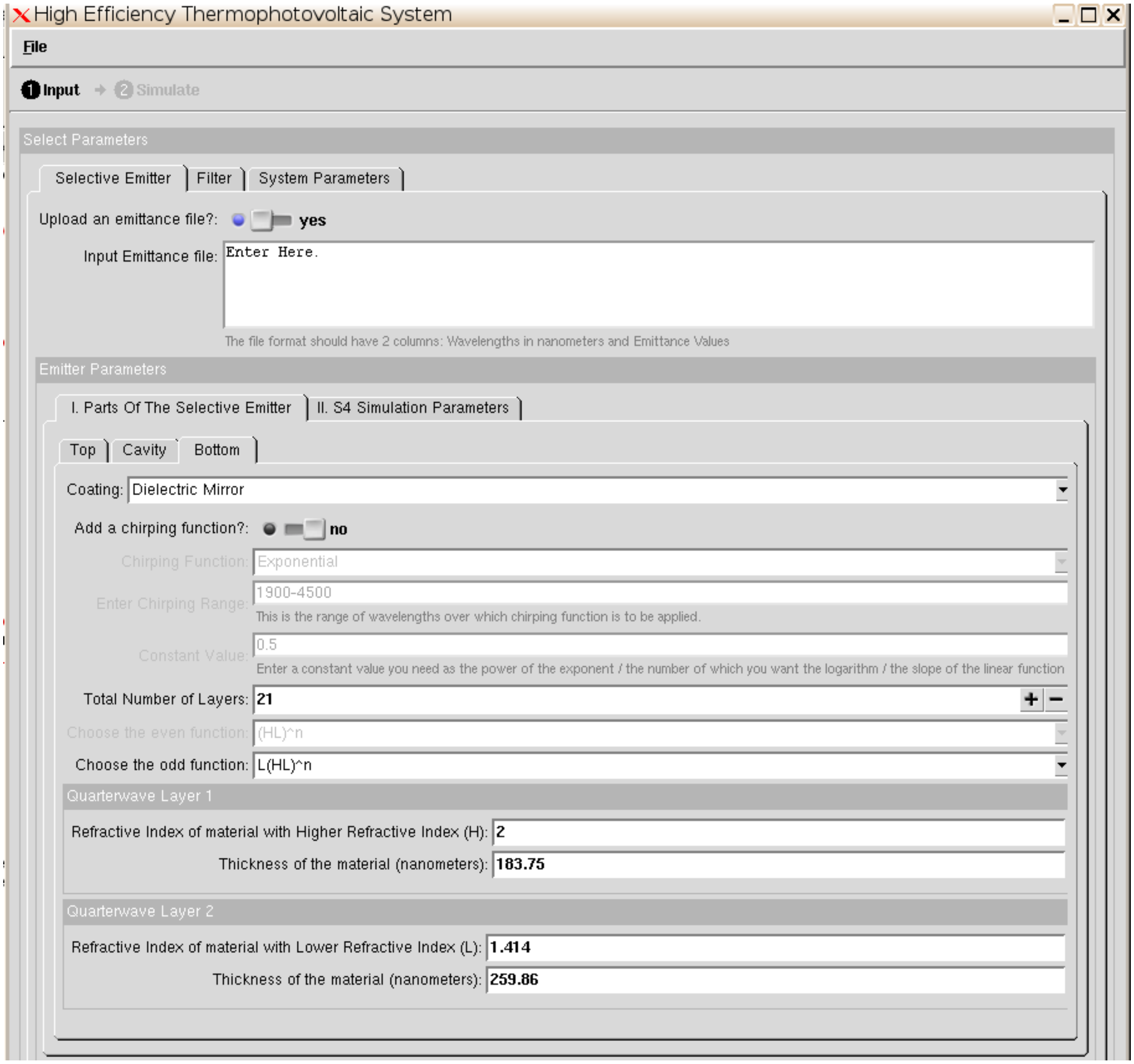
$$\bar{\epsilon}(T) = \frac{\int_0^{\infty} d\lambda\, \epsilon(\lambda) I_{BB}(\lambda, T)}{\sigma T^4}$$

nanoHUB.org was used to develop a graphical user interface called TPXsim. The tool allows the user to simulate thermophotovoltaic cells at the system level. NanoHUB.org is a website that supports simulation and learning especially for nanoscale level science and technology.

2.2 GUI simulation tool description

The graphical user interface (GUI) associated with the TPXsim tool on nanoHUB.org allows the user to set up proper emitter, filter and system parameters required for simulations. As shown in Fig. 1, there are tabs to set up appropriate parameters and designs for each component.

For the emitter part, the user may input an emittance file, or in other words, a list of emittance values against wavelengths. Alternatively, the user can enter parameters for the emitter. There are two tabs, one is for parts of the emitter, which includes options for top layer, middle layer and bottom layer specifications and the other for S4 simulation parameters.



Upload an emittance file?: yes

Input Emittance file: Enter Here.

The file format should have 2 columns: Wavelengths in nanometers and Emittance Values

Coating: Dielectric Mirror

Add a chirping function?: no

Chirping Function: Exponential

Enter Chirping Range: 1900-4500

This is the range of wavelengths over which chirping function is to be applied.

Constant Value: 0.5

Enter a constant value you need as the power of the exponent / the number of which you want the logarithm / the slope of the linear function

Total Number of Layers: 21

Choose the even function: (HL)^n

Choose the odd function: L(HL)^n

Quarterwave Layer 1

Refractive Index of material with Higher Refractive Index (H): 2

Thickness of the material (nanometers): 183.75

Quarterwave Layer 2

Refractive Index of material with Lower Refractive Index (L): 1.414

Thickness of the material (nanometers): 259.86

Figure 1. Graphical user interface for TPXsim on nanoHUB.org (https://nanohub.org/tools/tpxsim/).

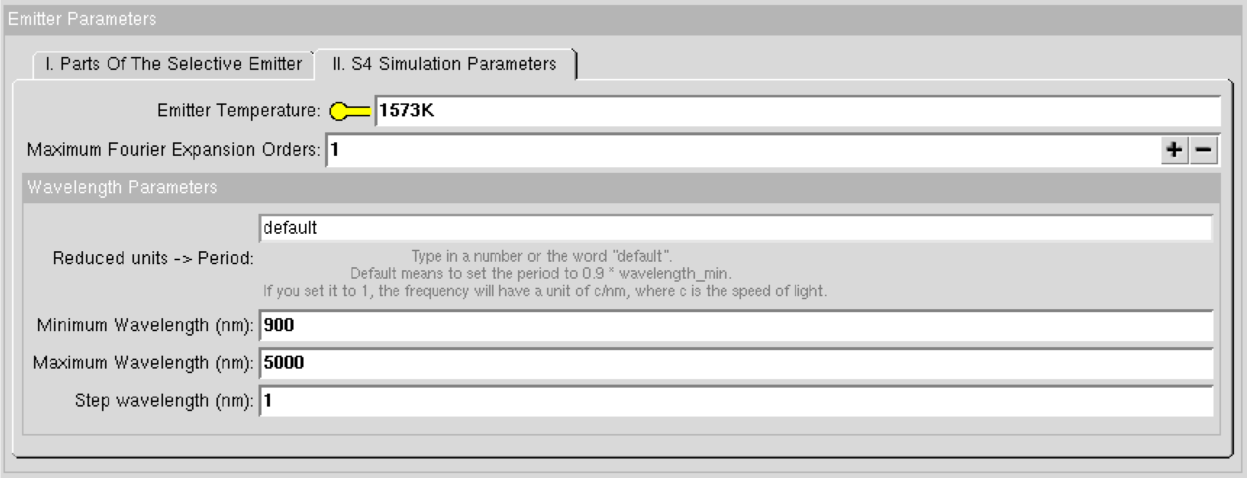
For the top part of the emitter, there are options for either adding an anti-reflection layer or a dielectric stack. As the name suggests, anti-reflection layer prevents reflection of any incoming radiation and thus help in maximizing the amount of radiation on the emitter. There are options to choose the total number of layers needed. Also there is an option to add chirping. The user can also select the function for chirping. Available options are exponential, logarithmic, and linear. There is an addition flexibility of choosing a context-dependent constant value. In case of exponential function, this is the exponent, in case of logarithmic function, this is the number of which the logarithm is being used. Similarly, in case of linear function, it is the value of the slope. In this way, a user can try out different values to find out cases with high efficiencies. The user can choose the number of layers to be even or odd and choose any corresponding structure type. For example, in the case of 5 layers, the layers can either vary as HLHLH or LHLHL. Similarly, in the case of 4 layers, they may vary as HLHL or LHLH. Also the user can then assign thicknesses and refractive index to the two alternating materials. In case of chirping, these thicknesses will be those of the layers closest to the cavity.

In case of the cavity part of the emitter, the user can choose the default value of ErAG as the material and in this case a file will be uploaded with real and imaginary part of dielectric constants varying with wavelengths in nanometers. The user can also upload other such files, to investigate whether other selective emitter materials could provide better efficiencies or cost-effectiveness.

The bottom layer of the emitter is similar to the top with an additional option for adding a substrate layer. For the substrate part of the thermophotovoltaic cell, the user may choose the default tantalum substrate, which automatically uploads a file with values of changing dielectric constants with wavelength of light. The dielectric constant is given as the square of the complex refractive index.

The values of dielectric constants vary considerably with wavelength in case of the substrate and cavity. However it can be assumed constant for dielectric materials used in the selective emitter.

There are other specifications that the user should provide for calculating the efficiency. The minimum and the maximum wavelength should correspond to the files uploaded in all the cases for calculating the efficiencies. Also, the minimum wavelength should be $1000\ \mu\text{m}\cdot\text{K}\ /T$ and max should be $6000\ \mu\text{m}\cdot\text{K}\ /T$ where T is the emitter temperature, based on the location of the blackbody peak, determined by Wien's law to be approximately $3000\ \mu\text{m}\cdot\text{K}\ /T$. Figure 2 shows how these parameters can be entered into the simulation



Emitter Temperature: 1573K

Maximum Fourier Expansion Orders: 1

Reduced units -> Period: default

Type in a number or the word "default".
Default means to set the period to 0.9 * wavelength_min.
If you set it to 1, the frequency will have a unit of c/nm, where c is the speed of light.

Minimum Wavelength (nm): 900

Maximum Wavelength (nm): 5000

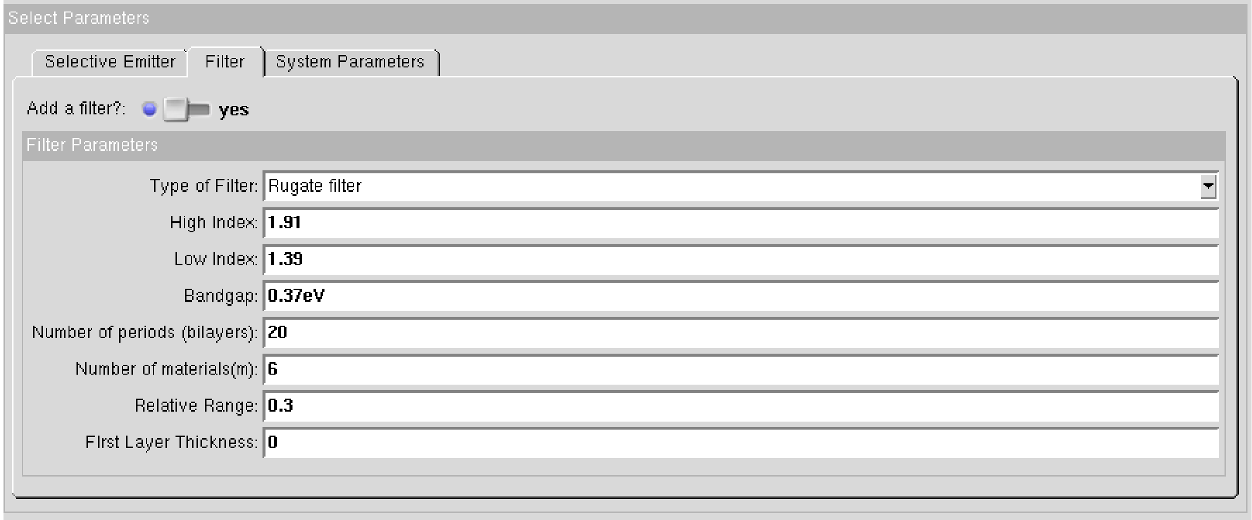
Step wavelength (nm): 1

Figure 2. Choosing the temperature, wavelength range, and S4sim parameters in TPXsim.

The user can input various other inputs such as photovoltaic bandgap and filter bandgap. The dark current density corresponds to the photovoltaic bandgap and should be calculated appropriately. Dark Current density can be calculated using the following formula:

$$J_D = 6e^{-40(PV_{bg}-0.534)}$$

The user can additionally choose a filter for recycling photons, which can be either a Rugate filter or a Quarterwave stack. The filter parameters can be entered as shown in Fig. 3.

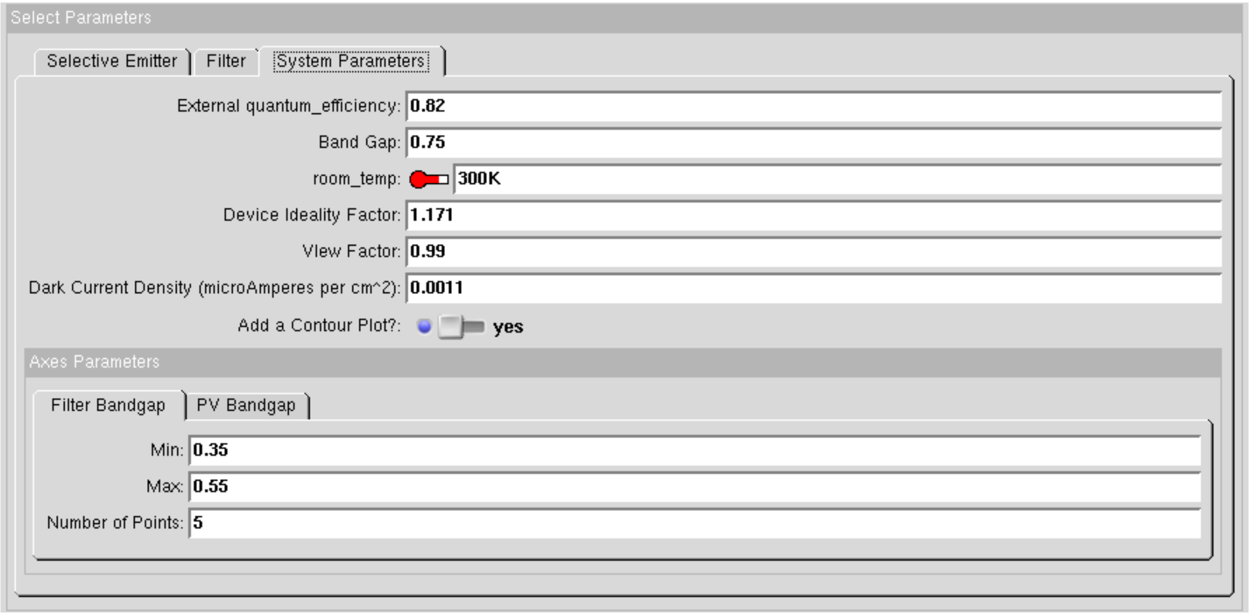


Add a filter?: yes

Type of Filter:	Rugate filter
High Index:	1.91
Low Index:	1.39
Bandgap:	0.37eV
Number of periods (bilayers):	20
Number of materials(m):	6
Relative Range:	0.3
FIrst Layer Thickness:	0

Figure 3. Selection of filter parameters in TPXsim.

There is an additional option for plotting the contour plot of efficiencies with changing PV bandgap and changing filter bandgap. The user can specify the minimum, maximum, the number of points on the two scales to find the best combination of PV bandgap and filter bandgap yielding maximum efficiency. Figure 4 shows the contour plot radio button toward the bottom; when enabled, it also allows the user to adjust the PV and filter bandgap ranges plotted.



External quantum_efficiency: 0.82
Band Gap: 0.75
room_temp: 300K
Device Ideality Factor: 1.171
View Factor: 0.99
Dark Current Density (microAmperes per cm^2): 0.0011
Add a Contour Plot?: yes

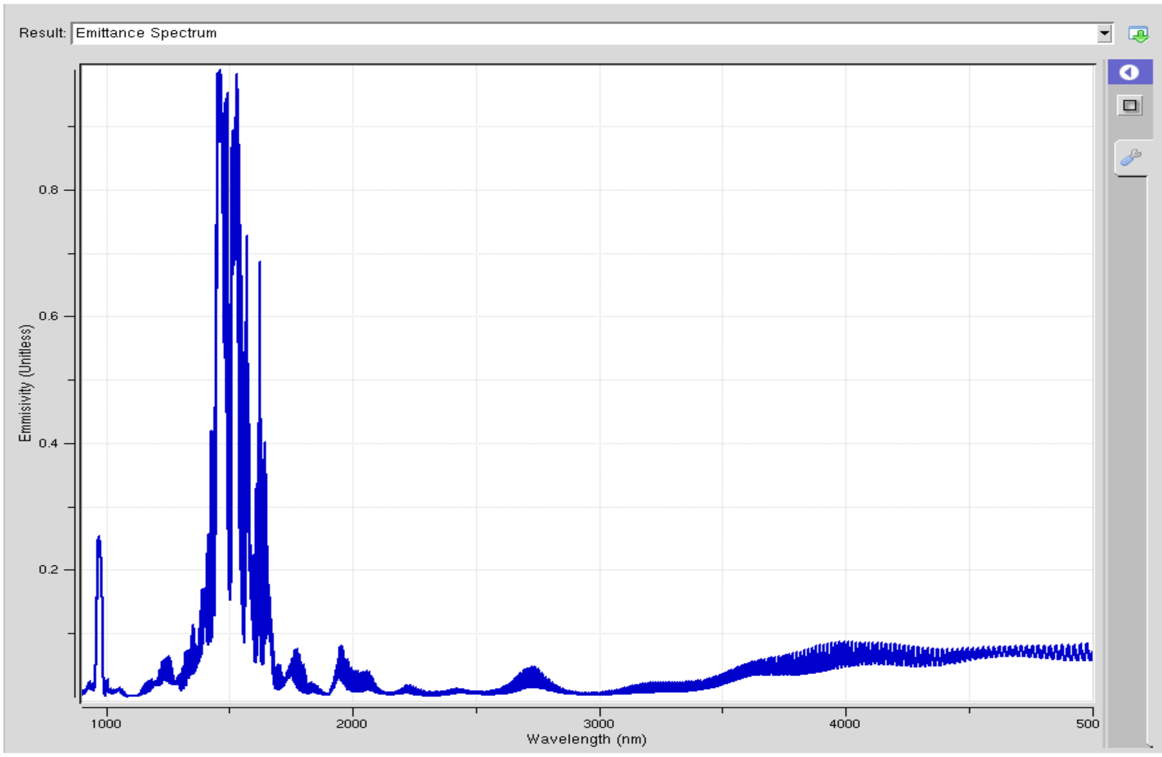
Min: 0.35
Max: 0.55
Number of Points: 5

Figure 4. Selection of thermophotovoltaic (TPV) cell and system parameters in TPXsim.

The development environment used is Rappture on nanoHUB.org. The GUI outputs an emittance plot for the emitter, a reflection spectrum for the filter, the average emissivity, the radiation efficiency, the overall thermophotovoltaic cell efficiency, a control file and the contour plot. The control file generated is scripted in LUA and is input into S4 tool on nanoHUB. S4 then generates absorption values which must equal the emittance in thermal equilibrium. Along with the blackbody curve at the appropriate temperature, these emittance values allow for calculation of the photovoltaic current. The intrinsic dark current associated with the photovoltaic diode, which runs in opposite direction to the photocurrent, is then subtracted from this photocurrent to yield the net current-voltage relation $J(V)$. This result can then be used to calculate the fill factor, open circuit voltage, and short circuit current, and thus the overall power output, which in turn yields the overall power conversion efficiency of the system.

3. Results

As shown in Fig. 5, the optimal emittance spectrum for erbium aluminum garnet enclosed by a pair of photonic crystal reflectors consists of a Q-matched peak at the 1.55 μm resonant wavelength, showing 100% emittance at that wavelength and zero emittance near long wavelength low energy wavelengths. Also, the reflectance spectrum of the filter shows that the longer wavelength photons are mostly reflected. From using contour plots like the one shown in Fig. 6, the maximum efficiency of 33.89% was found close to 0.37 eV for filter bandgap and 0.75 eV for PV bandgap. The contour plot also demonstrates the system is much more sensitive to the PV bandgap, with a tolerance on the order of 20 meV, compared to the filter bandgap, with a tolerance on the order of 200 meV. If a system within these tolerances were to be built and characterized experimentally, this would be an unprecedented thermophotovoltaic system efficiency.



Result: Emittance Spectrum

Figure 5. The emittance spectrum produced by an ErAG-based photonic emitter simulated in TPXsim shows almost 100% emission at the cavity resonant wavelength in the near-infrared region.

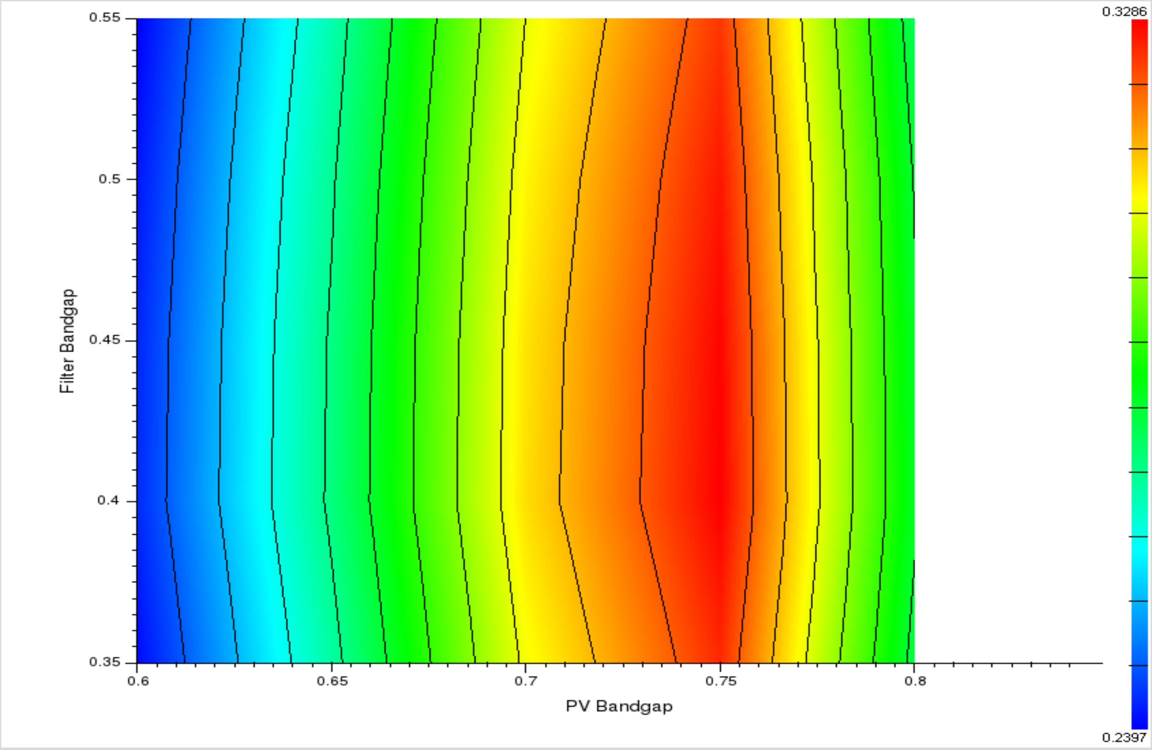


Figure 6. A contour plot of the TPV system efficiency with respect to PV Bandgap (x-axis) and filter bandgap (y-axis). The red region corresponds to the maximum efficiency values.

Right now, there is an ongoing research in the Birck Nanotechnology Center in Purdue University, where these simulations and predictions will be used to experimentally fabricate these structures and find their experimental efficiencies. If it is found to be experimentally feasible and viable, we may have the proposed selective emitter model incorporated in future thermophotovoltaic cells. Also, the tool on nanoHUB will be used to plot contour plots of efficiencies for many variations on this design, including different numbers of layers and dielectric materials, to help find improved design combinations for better efficiencies.

4. Conclusions

The present efficiency of a Thermophotovoltaic (TPV) cell limits the use of TPV technology for electricity generation process. Research experiments have consistently shown enhancement in the efficiency of these systems from various emitter-filter configurations. With the present emitter configuration we hope to achieve a world-record breaking efficiency of approximately 34%. The design attempts to enhance the emission of low-wavelength high-energy photons, thus increasing the number of photons in the above-bandgap energy level, consequently producing more electrical output. We developed a tool to allow the user to study and compare the emittance spectrum and efficiency output at various emitter configurations and PV cell bandgaps through simulations of chirped dielectric stack structures and coatings on a rare-earth ceramic substrate. The optimal efficiency of 33.89 % is achieved at filter bandgap of 0.37 eV and PV bandgap of

0.75eV. The research thus demonstrates the potential for unprecedented efficiencies for TPV cells. Future research in Purdue University will compare presented simulation results to experimental results.

Acknowledgments

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