Solar cell optimization

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Abstract

Solar power has the potential to generate much of the world's energy, but in order to reach this goal we must develop solar cells that are more efficient and cheaper to manufacture. In this paper we develop a technique for calculating and optimizing the power output of a solar cell, which we hope will allow researchers to create new and more efficient designs. We will first delve into the theory to explain how we developed our model, and then we will explain how to use the accompanying MATLAB software package to begin optimizing.

1 Optical waveguides

In this section I will develop some of the theory behind optical waveguides. We will eventually model solar cells as waveguides, so this theory is important for understanding how to maximize efficiency. I assume a little knowledge of differential equations and wave physics. It will be helpful to be able to code in MATLAB or another high-level language, so you can try some of the experiments out yourself, but is by no means necessary.

1.1 Derivation of formulae

We will begin by studying one-dimensional waveguides and two-dimensional electromagnetic plane waves. These waves have the form $e^{ik\mathbf{d}\cdot\mathbf{x}}$, where $\mathbf{x} = (x, y)$ and k is the wavenumber in radians per meter. k is related to the wavelength λ by $k = \frac{2\pi}{\lambda}$. κ is the spatial frequency in the x direction, or the x component of the wave vector $k\mathbf{d}$. The speed of light in a material is given by $v = \frac{c}{n}$, where c is the speed of light and n is the refractive index of the material. We suppose that we can separate the x and y components of the wave equation as follows:

$$\tilde{u}(x, y) = u(y)e^{i\kappa x}. \tag{1}$$

We also suppose that $\tilde{u}$ satisfies the equation

$$(\Delta + n^2k^2)\tilde{u} = 0. \tag{2}$$

Substituting (1) into (2), we obtain

$$(\partial_x^2 + \partial_y^2 + n^2k^2)u(y)e^{i\kappa x} = 0 \Rightarrow \partial_x^2 u(y)e^{i\kappa x} + \partial_y^2 u(y)e^{i\kappa x} + n^2k^2u(y)e^{i\kappa x} = 0$$

$$\Rightarrow -\kappa^2 u(y)e^{i\kappa x} + u''(y)e^{i\kappa x} + n^2k^2u(y)e^{i\kappa x} = 0 \Rightarrow u'' + (n^2k^2 - \kappa^2) = 0.$$

The general solution to this differential equation is

$$u(y) = c_1 e^{\sqrt{\kappa^2 - n^2k^2}\cdot y} + c_2 e^{-\sqrt{\kappa^2-n^2k^2}\cdot y}. \tag{3}$$

When $\kappa < nk$, the operand of the square root is negative and so we get complex exponentials, which equate with propagating waves in the y direction. When $\kappa > nk$, we get real-valued exponentials and we select the sign that gives decaying waves, or evanescent waves, since we do not want the waves to grow as they travel. When $\kappa = nk$, the differential equation reduces to $u'' = 0$, whose solution is $u(y) = a + by$.

We will now consider a one-dimensional domain along the y-axis, which we split into three regions. In the left-hand region the refractive index is n_0, in the middle it is n_1, and on the right it is n_2. In the left and right regions, we want the wave to decay when $\kappa > n_i k$, and we want the wave to propagate outwards when $\kappa < n_i k$. If we let $\alpha_i = \sqrt{n_i^2k^2 - \kappa^2}$ for $i = 0, 1, 2$, from (13) we determine that

$$u(y) = c_1 e^{-i\alpha_0 y} \tag{4}$$

in the left region. In the middle region,

$$u(y) = \begin{cases} c_2 e^{i\alpha_1 y} + c_3 e^{-i\alpha_1 y}, & \text{if } \kappa \neq n_1 k \\ c_2 + c_3 y, & \text{if } \kappa = n_1 k \end{cases} \tag{5}$$

and in the right region,

$$u(y) = c_4 e^{i\alpha_2 y} \tag{6}$$

In the transverse-electric (TE) case, we need u and u' to be continuous at the boundaries of the three regions. This means that at $y = 0$, $u_0(y) = u_1(y)$ and $u_0'(y) = u_1'(y)$, and at $y = a$, $u_1(y) = u_2(y)$ and $u_1'(y) = u_2'(y)$. When $\kappa = n_1 k$, we obtain the system of equations

$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -i\alpha_0 & 0 & -1 & 0 \\ 0 & 1 & a & -e^{i\alpha_2 a} \\ 0 & 0 & 1 & -i\alpha_2 e^{i\alpha_2 a} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

When $\kappa \neq n_1 k$,

$$\begin{pmatrix} 1 & -1 & -1 & 0 \\ -i\alpha_0 & -i\alpha_1 & i\alpha_1 & 0 \\ 0 & e^{i\alpha_1 a} & e^{-i\alpha_1 a} & -e^{i\alpha_2 a} \\ 0 & i\alpha_1 e^{i\alpha_1 a} & -i\alpha_1 e^{-i\alpha_1 a} & -i\alpha_2 e^{i\alpha_2 a} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

We want nontrivial vectors in the null space of the 4×4 matrix, i.e. constants c_1, c_2, c_3, and c_4 for which the system of equations has a solution. If we can find such constants, then we can construct the wave across the whole domain. We know that there will be nontrivial vectors in the null space of a matrix A if $\det(A) = 0$. We denote the 4×4 matrix from the above systems of equations by A. In MATLAB, we can find where $\det(A) = 0$ by doing an `imagesc` of $\log|\det(A)|$ over some range of k and κ. A sample plot is shown in figure 1. Where the plot is more negative (i.e. more blue), the determinant is small and the values of k and κ are close to the values where there exists a nontrival vector in the null space of A.

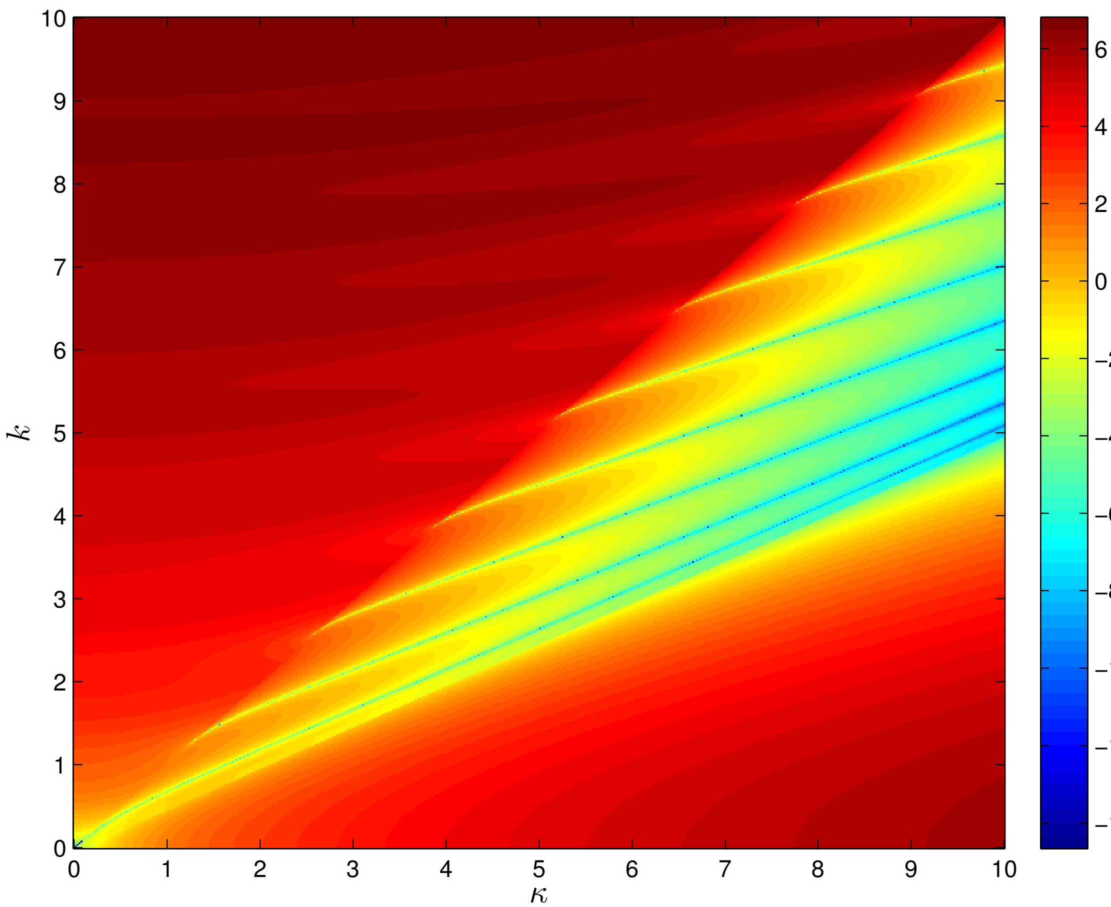

Figure 1: `imagesc` of $\det(A)$ for $n_0 = 1$, $n_1 = 2$, $n_2 = 1$, $a = 1.4$, $0 \leq k \leq 10$, $0 \leq \kappa \leq 10$ for TE case.

In this case $n_0 = n_2 = 1$, which we can see manifested in the plot by the line at $\kappa = 1k = n_0 k$. Above this line, called the light line, $\kappa < n_0 k$ and $\kappa < n_2 k$, so waves propagate outwards from the middle region. Below the light line, the waves decay exponentially outside the middle region. This means that the waves are trapped in the middle region. We also see a red triangle in the lower-right corner of the plot. This region has no physical meaning. When $\kappa > n_1 k$, the wave cannot exist, since then the speed of the wave in the x-direction would be greater than its total speed.

Figure 2 shows a sample wave located from the plot. $k = 7.76$ and $\kappa = 9.525$. y is along the horizontal axis and $u(y)$ is along the vertical axis. We can see that $u(y)$ decays exponentially outside of the middle region, as desired for $\kappa > n_0 k$ and $\kappa > n_2 k$. We notice that the values of k and κ correspond with the 6th streak of low determinant values in the plot, and that the wave has 6 half-waves in the middle region. We refer to resonances in this streak as being in the 6th mode.

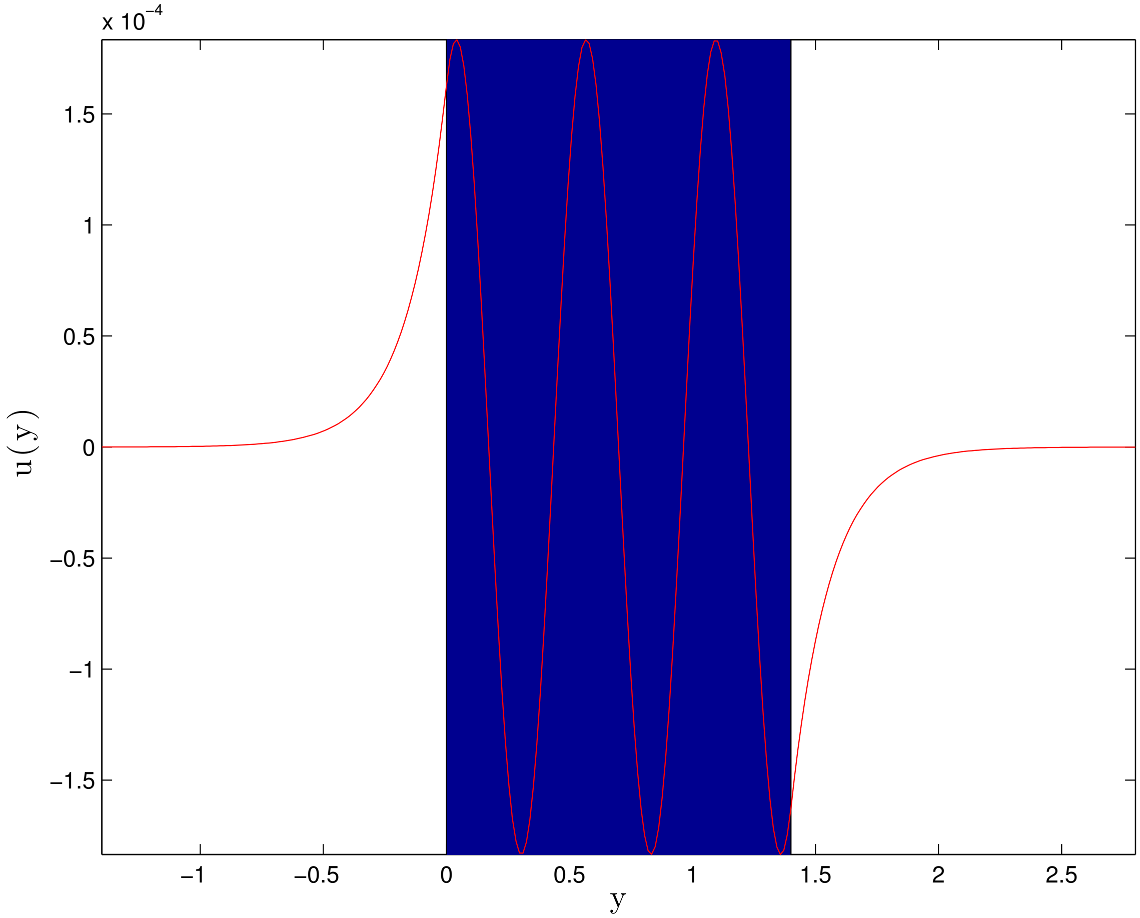

Figure 2: Plot of TE wave at $k = 7.76$ and $\kappa = 9.525$ (blue region is waveguide).

In the transverse-magnetic (TM) case, we need u and $\frac{u'}{n_i^2}$ to be continuous. This means that at $y = 0$, $u_0(y) = u_1(y)$ and $\frac{u_0'(y)}{n_0^2} = \frac{u_1'(y)}{n_1^2}$, and at $y = a$, $u_1(y) = u_2(y)$ and $\frac{u_1'(y)}{n_1^2} = \frac{u_2'(y)}{n_2^2}$. The systems of equations will be the same as for the TE case, except we divide A_{21} by n_0^2; A_{22}, A_{23}, A_{42}, and A_{43} by n_1^2; and A_{44} by n_2^2. We again do an `imagesc` over k and κ looking for nontrivial vectors in the null space, and obtain a plot like figure 3.

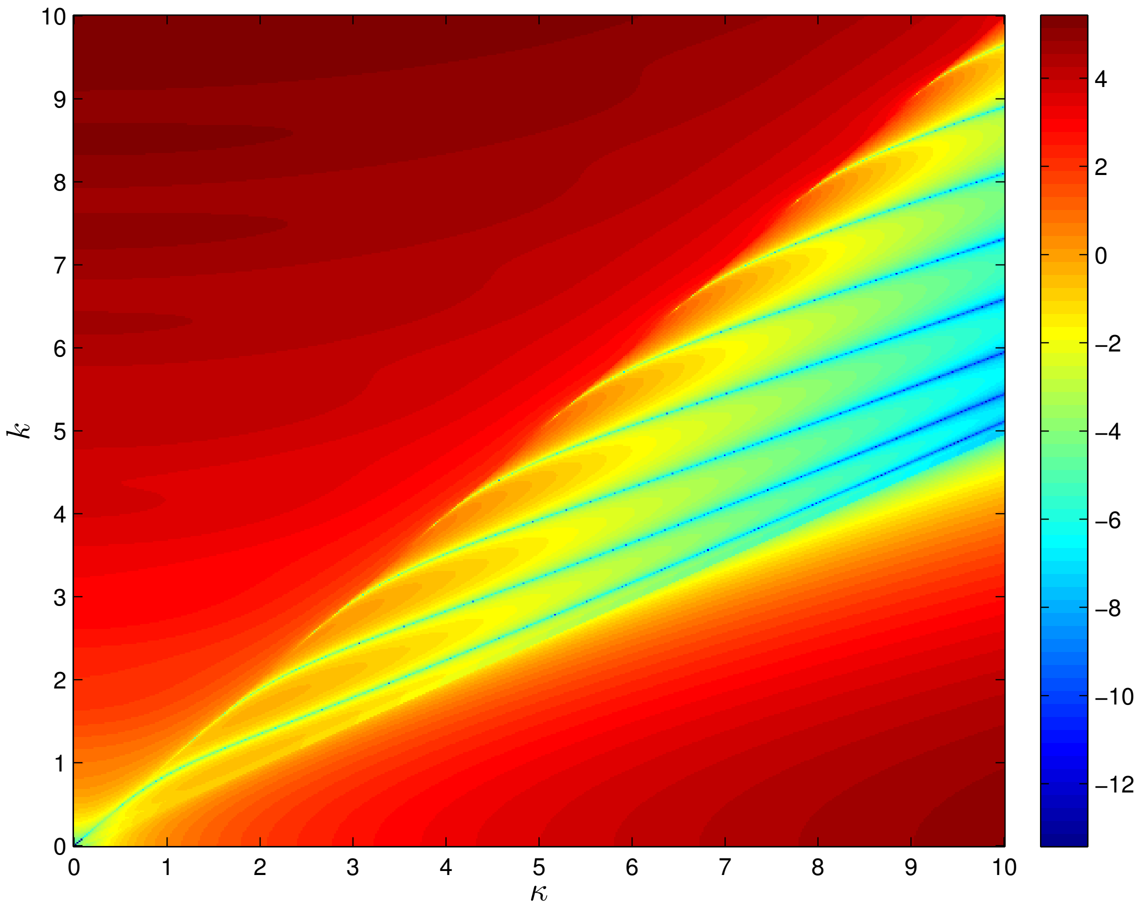

Figure 3: `imagesc` of $\det(A)$ for $n_0 = 1$, $n_1 = 2$, $n_2 = 1$, $a = 1.4$, $0 \leq k \leq 10$, $0 \leq \kappa \leq 10$ for TM case.

The plot is very similar to the TE case, and all the same analysis holds.

These plots give us a general idea of the values of k and κ for which the determinant is zero. We can find exact zeros by plotting the dispersion curves of the matrix, i.e. fixing k and then sweeping over the range of κ values we want to look at. To do this we make use of MPSpack, Alex Barnett and Timo Betcke's MATLAB toolbox. (Download the toolbox at http://code.google.com/p/mpspack/ and add the directory to the path). First we take a specific k value and we create a function $f(\kappa)$ that outputs the singular value decomposition of A with given k and input κ. Then we call evp.gridminfit (MPSpack function) with parameters f and the values of κ we want to sweep over. The first value returned is an array of the κ values which, with the given k, specify zeros of $\det(A)$. We can do this for as whatever range of k and κ values we like—figure 4 shows one possible plot of dispersion curves.

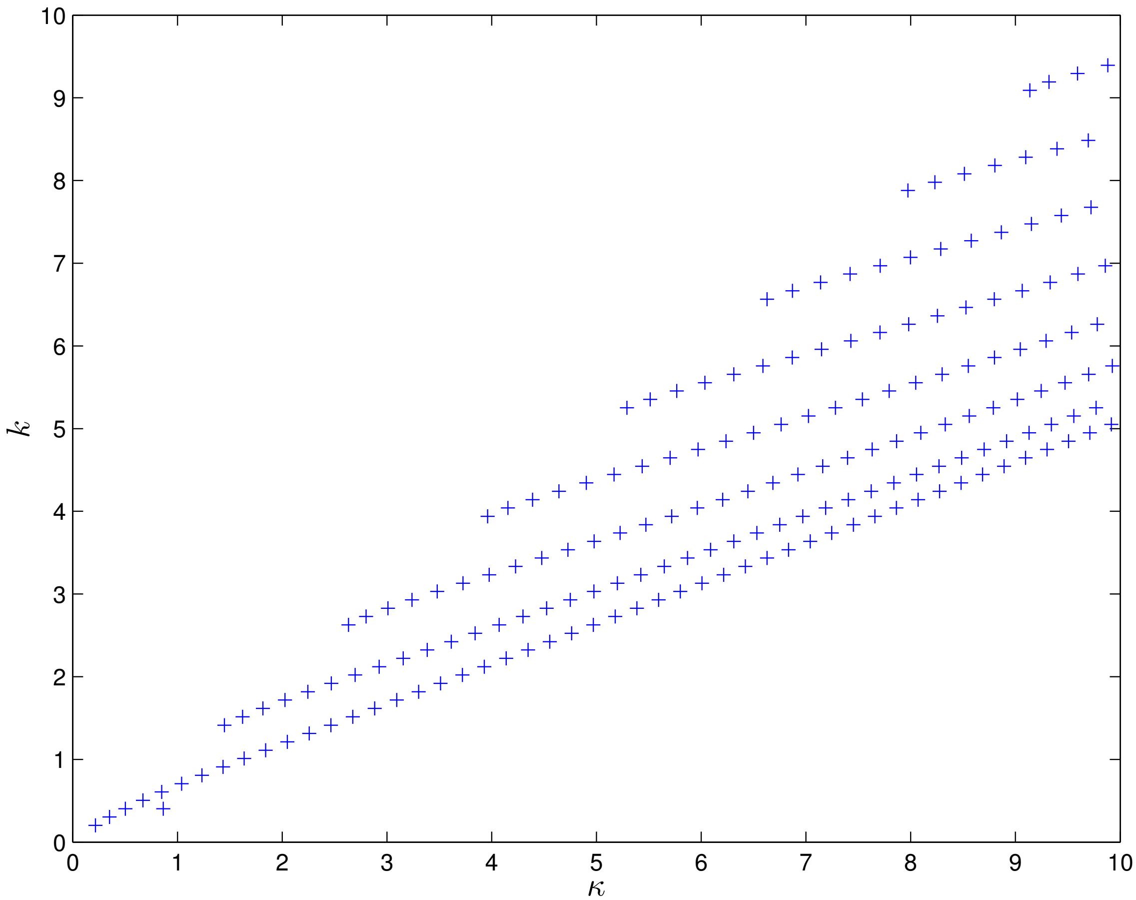

Figure 4: Dispersion curves of zeros of $\det(A)$ for $n_0 = 1$, $n_1 = 2$, $n_2 = 1$, $a = 1.4$, $0 \leq k \leq 10$, $0 \leq \kappa \leq 10$ for TE case.

1.2 Incident light

So far we have only studied the case where there is a wave is propagating along the waveguide and decaying on either side, which corresponds to $\kappa > k$. We now consider the case where there is an incident wave coming in from one side: part of the incident wave enters the waveguide and part of it reflects off and travels in the direction whence it came. This phenomenon is known as scattering. We can build this into our model by adding a propagating wave to the first region. This incident wave propagates towards the waveguide with constant amplitude. Again we let $\alpha_i = \sqrt{n_i^2 k^2 - \kappa^2}$ for $i = 0, 1, 2$. From (13), and taking into account the incident wave, we define

$$u(y) = e^{i\overline{\alpha_0} y} + c_1 e^{-i\alpha_0 y} \tag{7}$$

in the left region. In the middle region,

$$u(y) = \begin{cases} c_2 e^{i\alpha_1 y} + c_3 e^{-i\alpha_1 y}, & \text{if } \kappa \neq n_1 k \\ c_2 + c_3 y, & \text{if } \kappa = n_1 k \end{cases} \tag{8}$$

and in the right region,

$$u(y) = c_4 e^{i\alpha_2 y} \tag{9}$$

The boundary conditions for the TE case are the same as above, so when $\kappa = n_1 k$, we obtain the system of equations

$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -i\alpha_0 & 0 & -1 & 0 \\ 0 & 1 & a & -e^{i\alpha_2 a} \\ 0 & 0 & 1 & -i\alpha_2 e^{i\alpha_2 a} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} -1 \\ -i\overline{\alpha_0} \\ 0 \\ 0 \end{pmatrix}$$

When $\kappa \neq n_1 k$,

$$\begin{pmatrix} 1 & -1 & -1 & 0 \\ -i\alpha_0 & -i\alpha_1 & i\alpha_1 & 0 \\ 0 & e^{i\alpha_1 a} & e^{-i\alpha_1 a} & -e^{i\alpha_2 a} \\ 0 & i\alpha_1 e^{i\alpha_1 a} & -i\alpha_1 e^{-i\alpha_1 a} & -i\alpha_2 e^{i\alpha_2 a} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} -1 \\ -i\overline{\alpha_0} \\ 0 \\ 0 \end{pmatrix}$$

We seek k and κ such that the norm of the vector

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

is large. If the norm is large, then c_2 and c_3 will be large and the value of u will be large in the waveguide. We can again do an `imagesc` over a range of values, as seen in figure 5.

Figure 6 shows a wave along the second resonance curve. Notice how the value of u is much higher inside the waveguide than outside, and how there are two half-waves, again corresponding to the second mode.

Figure 7 is the same wave as figure 6 with the periodicity in the x direction reintroduced, as in (1). The y-axis is now vertical, so the waveguide is horizontal. The value of $u(y)$ is given by the color bar on the right.

We introduce time to the plot by multiplying all values by $e^{-i\omega t}$, where $\omega = ck$ and c is the speed of light. By incrementing the value of time we can animate the wave plots. In figure 7, the waves in the top region would propagate downwards toward the waveguide and the waves in the bottom region would propagate downwards away from the waveguide. The waves in the waveguide would propagate to the right.

1.3 Mirror-backed waveguide

So far we have been studying a three-layer system consisting of two outer regions and an inner waveguide. We now turn to a four-layer system with an outer region, a cladding layer, an active layer, and a perfect electric conductor (PEC). The cladding and active layers together comprise the waveguide. The PEC is a perfect mirror and will reflect all electromagnetic waves at its boundary, so we don't need an equation for the propagation of light inside it.

$$u(y) = \begin{cases} e^{\alpha_0 y} + c_1 e^{\alpha_0 y}, & \text{if } \kappa > n_0 k \\ e^{\alpha_0 y} + c_1 e^{-\alpha_0 y}, & \text{if } \kappa < n_0 k \\ c_1, & \text{if } \kappa = n_0 k \end{cases} \tag{10}$$

in the outer region. In the cladding layer,

$$u(y) = \begin{cases} c_2 e^{\alpha_1 y} + c_3 e^{-\alpha_1 y}, & \text{if } \kappa \neq n_1 k \\ c_2 + c_3 y, & \text{if } \kappa = n_1 k \end{cases} \tag{11}$$

and in the active layer,

$$u(y) = \begin{cases} c_4 e^{\alpha_2 y} + c_5 e^{-\alpha_2 y}, & \text{if } \kappa \neq n_2 k \\ c_4 + c_5 y, & \text{if } \kappa = n_2 k \end{cases} \tag{12}$$

Applying the boundary conditions for the TE case and computing the norm of the vector solution, we obtain a plot like figure 8.

Figure 9 shows a resonance of this four-layer system with PEC. The top layer is the outer region, the middle is the cladding, the bottom is the active layer, and the PEC begins at the bottom edge of the plot. The κ and k values were taken from the second broad band of red lines in figure 9, and we can see that this corresponds to the second mode since there are two half-waves in the active layer in figure 10.

1.4 Arbitrary waveguides

In the previous sections we showed how to solve for the coefficients of the wave equation in a three-layer waveguide. We will now show how to find the coefficients in an arbitrary-layer waveguide, for any frequency and angle of incident light, and for both the transverse-electric and transverse-magnetic modes.

Consider an m-layer two-dimensional waveguide, i.e., m layers infinite in length but finite in width sandwiched by free space on one side and an infinite substrate on the other. The substrate can be a mirror or an infinitely thick layer of constant refractive index. For convenience we will refer to free space as layer 0 and the substrate as layer $m+1$. If we suppose that the waveguide is infinite in the x direction and layered in the y direction, the y component of the wave equation in each layer is given by

$$u_i(y) = c_{i,1} \cdot e^{i\alpha_i y} + c_{i,2} \cdot e^{-i\alpha_i y} \tag{13}$$

for $i = 1, 2, ..., m$. We define $\alpha_i = \sqrt{n_i^2 k^2 - \kappa^2}$ for $i = 0, 1, 2, ..., m+1$, where $n_0 = 1$ and n_1,...,n_{m+1} are given. $c_{i,1}$ and $c_{i,2}$ are constants that determine the amplitude of the wave in the layer. The wave equation in the substrate is

$$u_{m+1}(y) = \begin{cases} 0, & \text{if the substrate is a mirror} \\ c_{m+1,1} \cdot e^{i\alpha_{m+1} y}, & \text{otherwise} \end{cases} \tag{14}$$

and in free space the wave equation is

$$u_0(y) = e^{\overline{\alpha_0} y} + c_{0,1} \cdot e^{-i\alpha_0 y} \tag{15}$$

where $\alpha_0 = \sqrt{k^2 - \kappa^2}$. The first term in (15) is the incident light going into the waveguide.

In the transverse-electric (TE) case, u and u' must be continuous at the boundaries of the m layers, free space, and the substrate. Thus we require $u_i(y_i) = u_{i+1}(y_i)$ and $u_i'(y_i) = u_{i+1}'(y_i)$ for $i = 0, 1, ..., m+1$, where y_i is the y value of the boundary between layers i and $i+1$. In the tranverse-magnetic (TM) case, u and $\frac{u'}{n_i^2}$ must be continuous at the boundaries, so we replace the condition that $u_i'(y_i) = u_{i+1}'(y_i)$ with $\frac{u_i'(y_i)}{(n_i)^2} = \frac{u_{i+1}'(y_i)}{(n_{i+1})^2}$.

These requirements give us a system of $2m+2$ equations which we can use to solve for the coefficients $c_{0,1}, c_{1,1}, c_{1,2}, c_{2,1}, c_{2,2}, ..., c_{m,1}, c_{m,2}, c_{m+1,1}$. This code is implemented in solveMultilayer.m.

2 Applications to solar cells

Calculating the coefficients of the wave equation is all well and good, but in order to optimize for solar cell efficiency we must determine how much light is actually being absorbed by the solar cell, which we are modeling as a waveguide. If we we denote the incident flux by F_{in} and the outgoing flux by F_{out}, the absorbance of the solar cell, or the fraction of radiation absorbed, is given by

$$\frac{F_{in} - F_{out}}{F_{in}}.$$

Letting $k_{y,in} = \alpha_0$ denote the frequency of the incident light in the y direction, $F_{in} = k_{y,in}$. To calculate the outgoing flux, we must calculate $k_{y,out}$, the frequency of the outgoing light in the y direction in the substrate, because $F_{out} = k_{y,in} \cdot |c_{0,1}|^2 + k_{y,out} \cdot |c_{m+1,1}|^2$. In the TE case $k_{y,out} = \alpha_{m+1}$ and in the TM case $k_{y,out} = \frac{\alpha_{m+1}}{(n_{m+1})^2}$. With this information we can calculate the absorbance of a given waveguide structure, which is also implemented in solveMultilayer.m.

2.1 Optimization

With the technique outlined above we can begin to optimize designs over the number and thickness of layers and the choice of material. It's important to choose the right material because materials with different refractive indices have very different absorbance levels.

To simulate an actual solar cell we must specify the active layer, which is the layer of silicon that will absorb photons and generate electricity when sandwiched between two conductive oxide layers of indium tin oxide (ITO). ITO has a refractive index of $2 + 0.6i$ at 500 nm. We can send in incident light at any frequency, look up the refractive index of silicon at that frequency (figure 10), and then calculate the absorbance of the solar cell. If we sweep across the solar spectrum and multiply absorbance and incoming photons at each frequency, we can integrate using Gaussian quadrature to find the total fraction of photons absorbed by the solar cell. We calculate the number of incoming photons at a given frequency as a function of the solar spectral irradiance (figure 11). This process is implemented in totalSpectralAbsorbance.m, which calculates the efficiency of an arbitrary solar cell design.

Now that we are able to calculate the efficiency of a given solar cell across the spectrum, we can begin plugging in different designs to find what works best. We must simply input the number of layers in the solar cell and each layer's thickness and refractive index and we can see how much of the solar energy will be absorbed. This process has been automated in optimize.m: simply input the number of layers, the index of the active layer, whether the solar cell is backed by a mirror or not, and some starting values, and you can find the optimum structure for an m-layer solar cell. For example, `[ds,ns,a] = optimize(2,true,2,[2,.0633],[1,1,1])` yields a local maximum absorbance of 0.4415 for a 2-layer mirror-backed solar cell with the second layer active. This absorbance is achieved when layer 1 is 2.2155 μm thick and has a refractive index of 1.4620, and the active layer of silicon is 0.0821 μm thick. Of course in addition to these two layers there is a pair of ITO layers sandwiching the silicon, in order to generate electricity.

3 Usage

To get started with the optimization software, you must first download Alex Barnett and Timo Betcke's MPSpack toolbox (download at http://code.google.com/p/mpspack/ and add the directory to the path). Below are a few functions and how to use them:

- `solveMultilayer(polarization, mirror, k, kappa, ds, ns)`

  Parameters:

  - polarization: 'te' or 'tm'
  - mirror: true or false
  - k: wavenumber of incident light
  - kappa: wavenumber of incident light in the x direction
  - ds: array of layer thicknesses
  - ns: array of refractive indices

  Usage: `[a,coeffs]=solveMultilayer('te', false, 8, 6, [.5,.2], [3,2+0.1*1i,1])`

  Output: absorbance and coefficients of the wave equation for each layer

- `totalSpectralAbsorbance(m, mirror, ix, ds, ns)`

  Paramaters:

  - m: number of layers in waveguide
  - mirror: true or false
  - ix: index of active layer
  - ds: array of layer thicknesses
  - ns: array of refractive indices

  Usage: `a=totalSpectralAbsorbance(2,true,3,[1.2,0.05],[3.4,2+0.6*1i])`

  Output: absorbance

- `optimize(m, mirror, ix, ds, ns)`

  Paramaters:

  - m: number of layers in waveguide
  - mirror: true or false
  - ix: index of active layer
  - ds: initial values of layer thicknesses
  - ns: initial values of of refractive indices

Usage: `[ds,ns,a] = optimize(2,true,2,[2,.0633],[1,1,1])`

Output: optimum layer thicknesses, refractive indices, and total absorbance of an m-layer solar cell

- `threelayergui(type, n0, n1, n2, a, kappa_min, kappa_max, k_min, k_max)`

  Parameters:

  - type: 'te' or 'tm'
  - n0: refractive index of layer 0
  - n1: refractive index of layer 1
  - n2: refractive index of layer 2
  - a: thickness of layer 1
  - kappa_min: minimum kappa value to sweep over
  - kappa_max: maximum kappa value to sweep over
  - k_min: minimum k value to sweep over
  - k_max: maximum k value to sweep over

  Usage: `threelayergui('te',3.5,1,3.5,1,0,10,0,10)`

  Output: Resonance plot of kappa vs. k for a three-layer waveguide. You can click on a point to see an animation of light traveling through the waveguide.

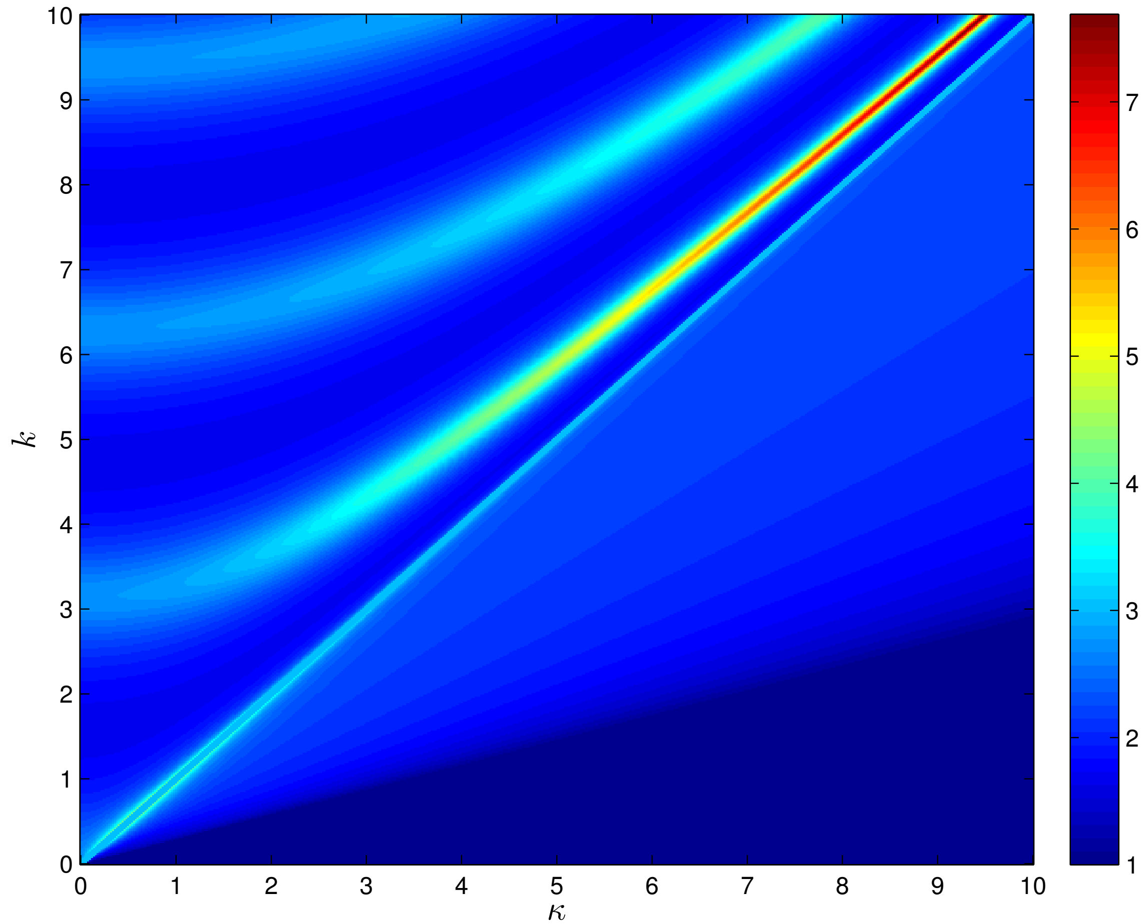

Figure 5: `imagesc` of norm of A with incident wave for $n_0 = 3.5$, $n_1 = 1$, $n_2 = 3.5$, $a = 1$, $0 \le k \le 10$, $0 \le \kappa \le 10$ for TE case.

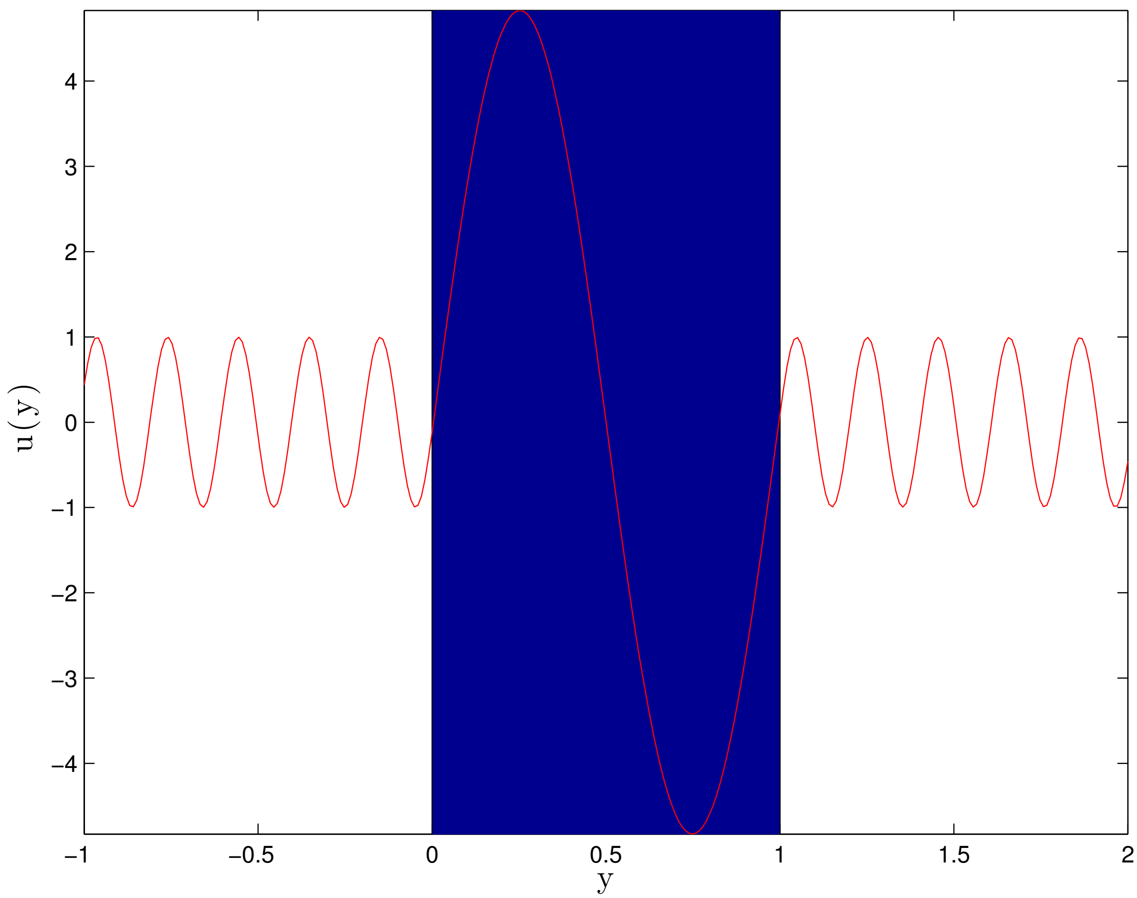

Figure 6: 1D plot of TE wave at $k = 9$ and $\kappa = 6.4$ with $n_0 = 3.5$, $n_1 = 1$, $n_2 = 3.5$, $a = 1$ (blue region is waveguide).

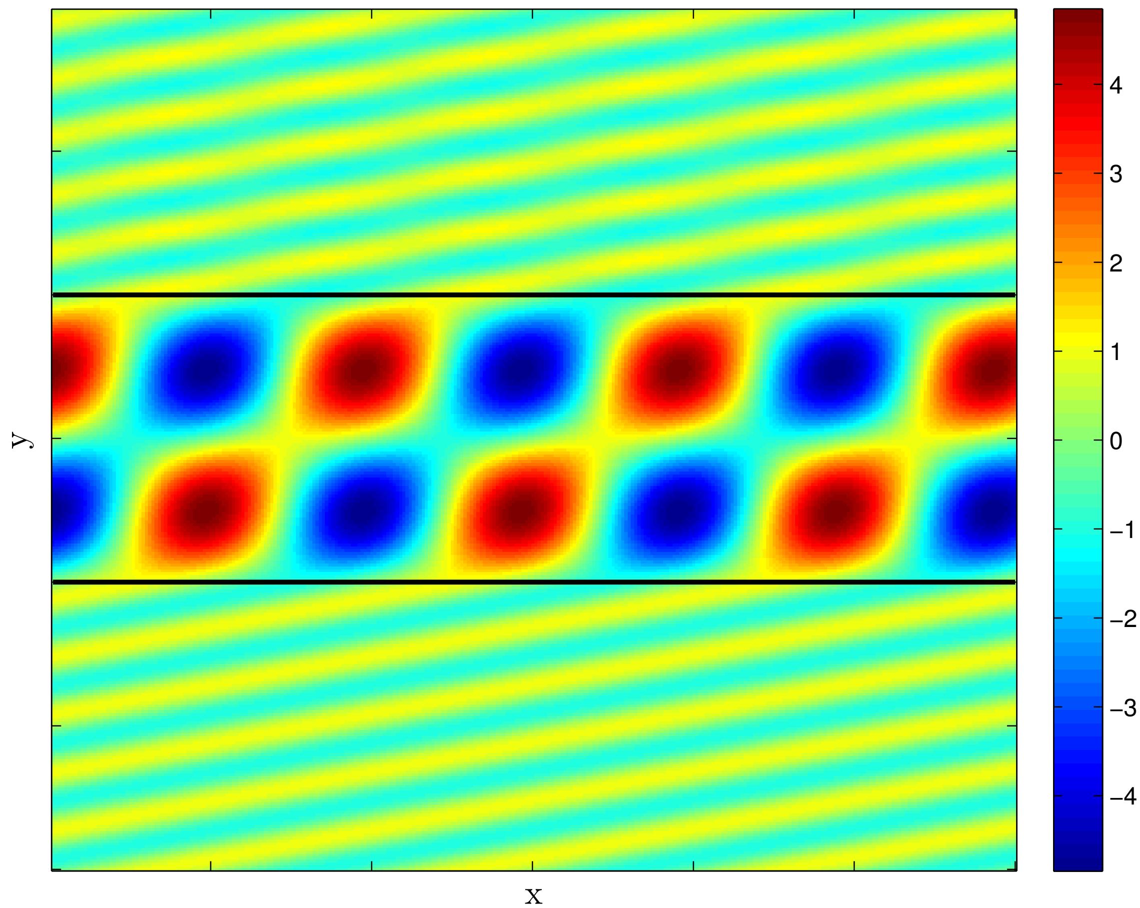

Figure 7: 2D plot of TE wave at $k = 9$ and $\kappa = 6.4$ with $n_0 = 3.5$, $n_1 = 1$, $n_2 = 3.5$, $a = 1$.

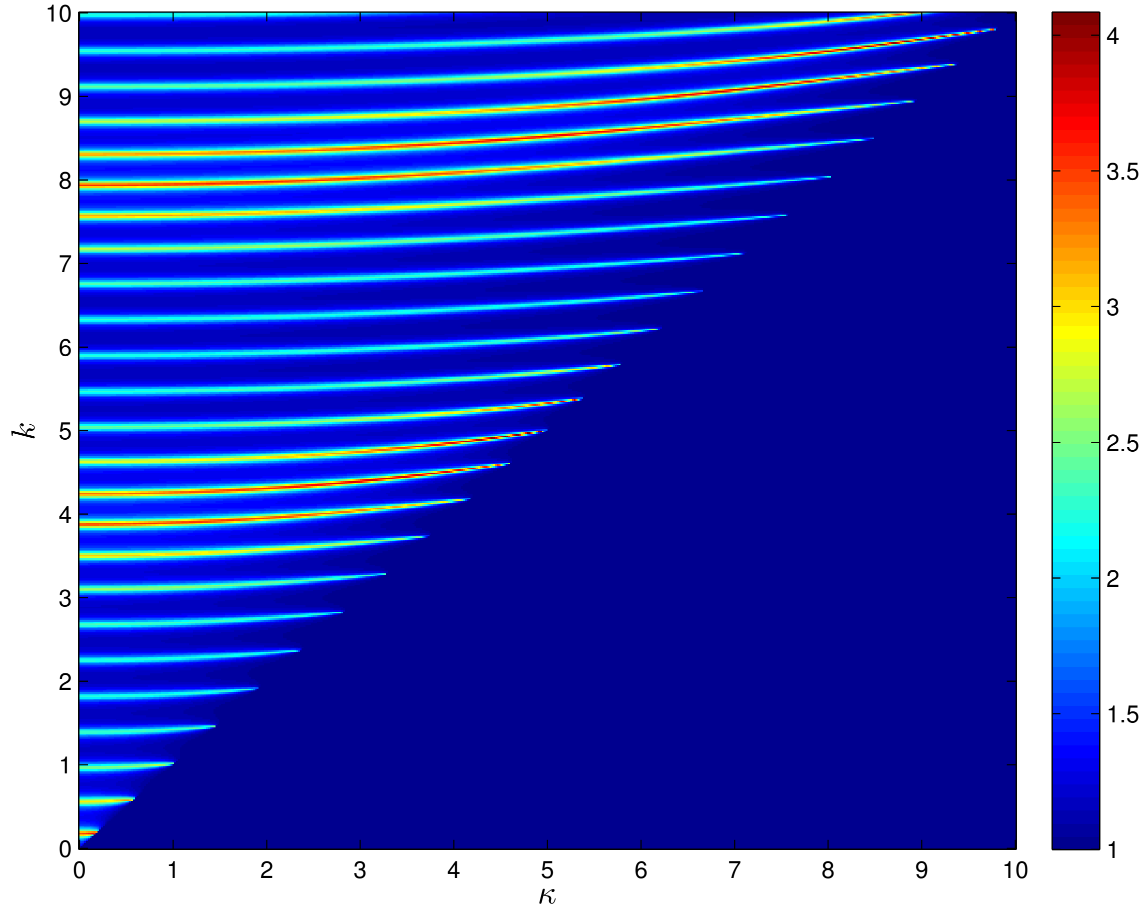

Figure 8: `imagesc` of norm of A with incident wave and PEC for $n_0 = 1$, $n_1 = \sqrt{12}$, $n_2 = \sqrt{2.5}$, $d_1 = 2$, $d_2 = 2.5$, $0 \leq k \leq 10$, $0 \leq \kappa \leq 10$ for TE case.

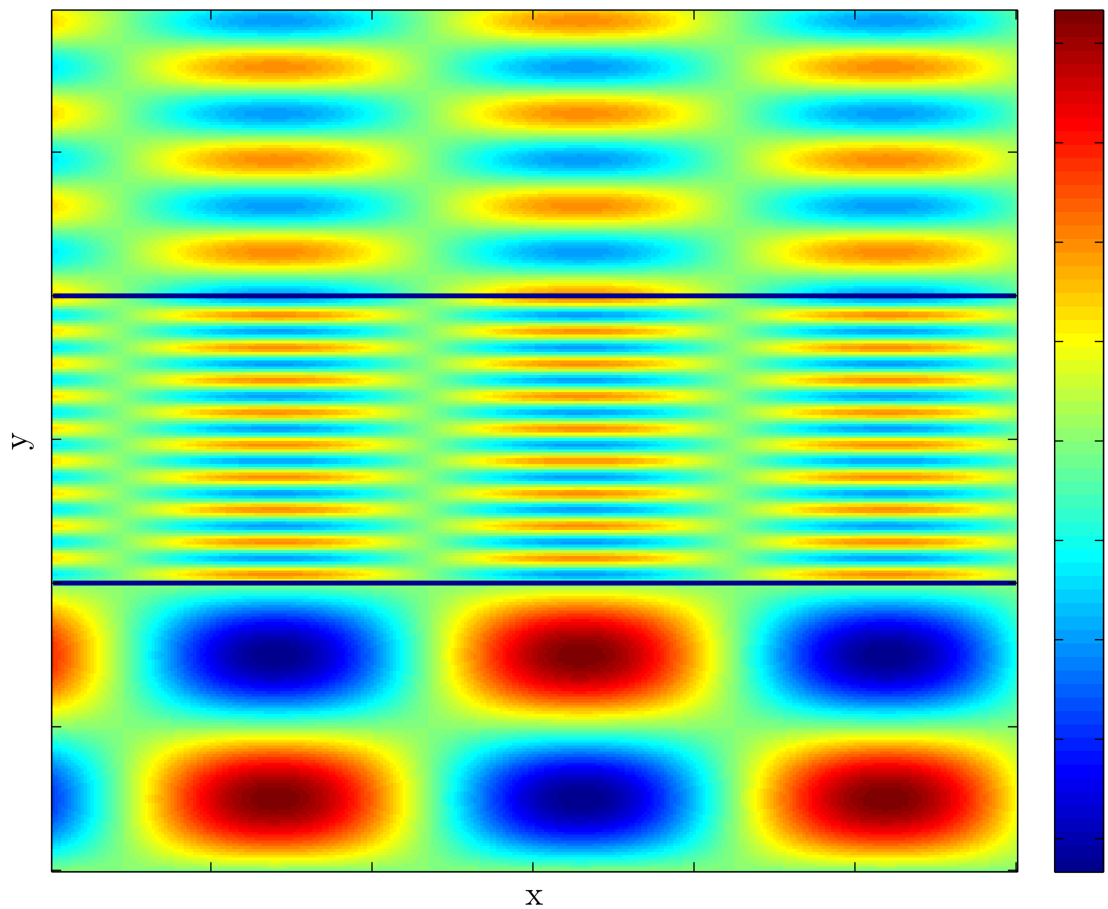

Figure 9: 2D plot of TE wave at $k = 7.98$ and $\kappa = 1.98$ with $n_0 = 1$, $n_1 = \sqrt{12}$, $n_2 = \sqrt{2.5}$, $d_1 = 2$, $d_2 = 2.5$.

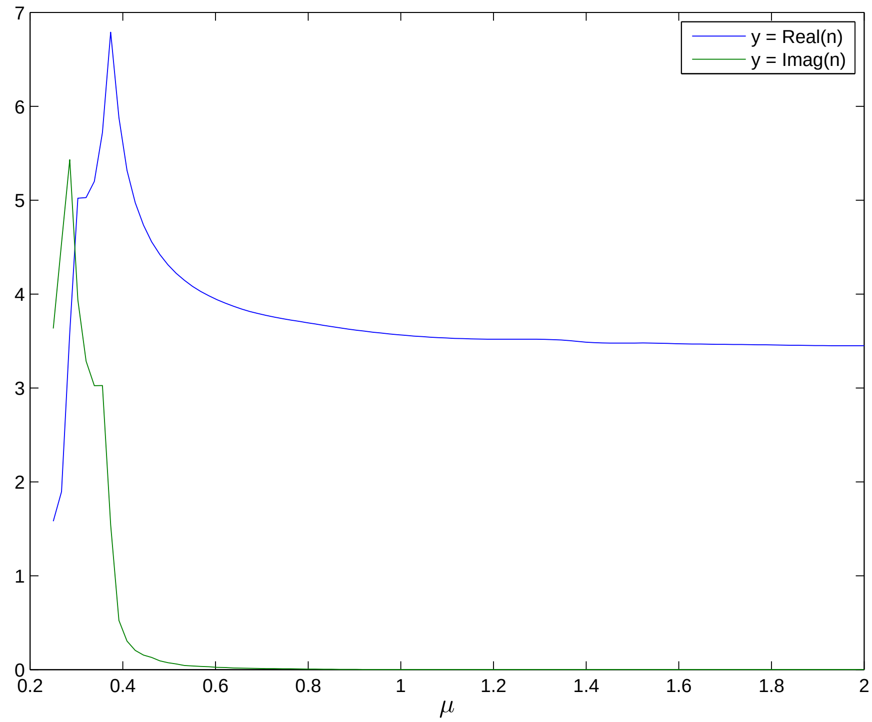

Figure 10: Real and imaginary parts of the refractive index of silicon (n) at various wavelengths

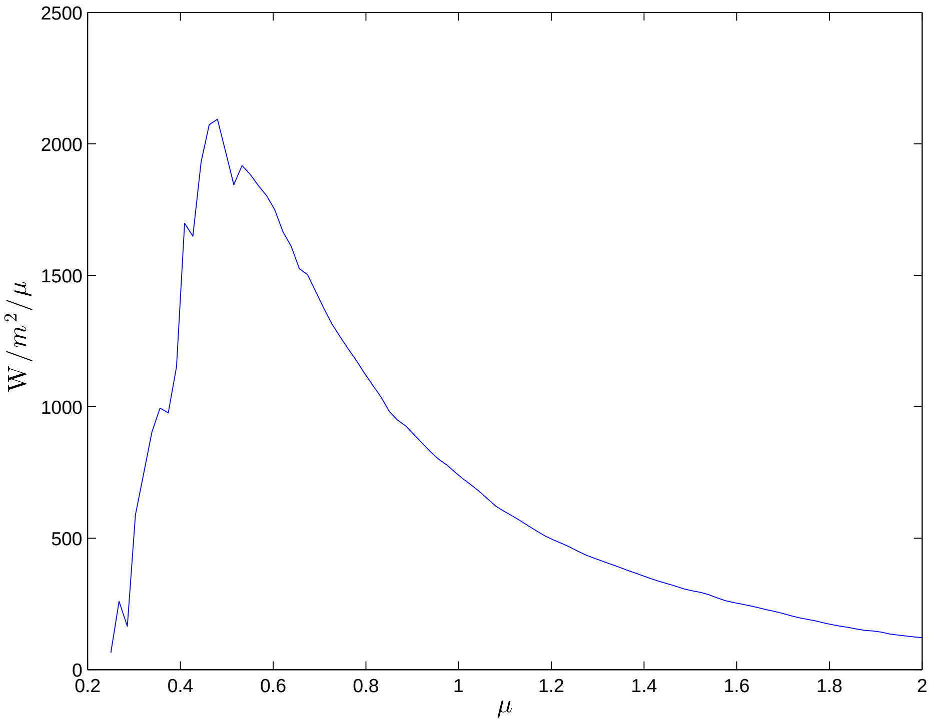

Figure 11: Wavelength vs. solar irradiance