Modeling of absorption and emission of light in semiconductor nanowires

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1 Introduction

1.1 The project

In this report we describe the interaction of light with an array of (nano) wires placed perpendicular on a substrate. This kind of surfaces have several kinds of applications depending on the size and material type of the nanowires. We are most interested in the arrays where the nanowire diameters is of the same dimensions as the wavelength of the incoming light. In this regime the nanowire arrays shows some very interesting characteristics which can have several applications, ranging from solar cells to pixels in an image.

1.2 Regimes

We can divide the interaction of light of wavelength λ with our nanowire surface in 3 different regimes[2].

$D >> \lambda$: in this regime we can use geometrical ray tracing optics to describe the interaction of light with the surface and the system can be solved very easily and will act as a classical surface. This is the most simple case, and for the purpose of this project also the most uninteresting case.

$D << \lambda$: In this regime we can use electrostatics to describe the system and solve the Laplace equations to get our solutions for the problem.

$D \approx \lambda$ In this regime we have to use nanophotonics, through the full Maxwell equations, to describe the system.

The nanowire surfaces that we will analyze are in the regime of the nanophotonics and the electrostatic regime. In those regimes we get very specific absorption for certain wavelengths.

1.3 Nano-wires application

Nanowires can be used to make high efficiency solar panels. A GaAs nano-wire array solar cell with an efficiency of 15.3 % was built by a team at Sol Voltaics[3]. Nanowire solar cell could reduce the cost and material consumption compared to the solar panels currently used in the industry. The panels can be more efficient and also contain less volume of expensive materials. Interaction between light and nano-wire is then presently studied in order to make those devices the most efficient possible.
Also surfaces with different colors are possible by using nano-wires of different diameters, since they absorb resonantly a wavelength that is chosen by tuning their diameter. [1]

2 The Program

The code is a numerical solver for the Maxwell equations that are of the family of PDE's. The program uses the scattering matrix method to obtain the solutions to the Maxwell equations[4].

2.1 Numerical errors

If we run the code for different sizes of the wave basis, we could see how the result converges, this could give us an estimation of the error. The method used is the scattering method. If we run the script for 5 different precision's (n corresponds to the size of the basis) we get:

precision n	T_n	R_n	$T_n - T_{n-1}$	$R_n - R_{n-1}$	T_n	R_n	$T_n - T_{n-1}$	$R_n - R_{n-1}$
8	−	−	−	−	0.3294	0.1270	0.0001	0.0007
7	−	−	−	−	0.3293	0.1263	0.0103	0.0110
6	−	−	−	−	0.3397	0.1353	0.0123	0.0081
5	0.8229	0.1770	0.0019	0.0030	0.3274	0.1272	0.0439	0.0403
4	0.8210	0.1800	0.0011	0.0012	0.2835	0.0869	0.0485	0.0328
3	0.8199	0.1812	0.0120	0.099	0.3320	0.1197	0.0528	0.0570
2	0.8078	0.1911	0.0230	0.0212	0.3848	0.1767	0.1851	0.0230
1	0.7849	0.2123	−	−	0.3355	0.1997	−	−

The parameters for the first set of values are [$\lambda = 1000nm\ period_{nanowires} = L_{nanowires} = 500nm$ and for the diameter 180nm], and for the second set only the $\lambda = 400nm$ is changed, both for normal incidence. for both set of specifications the method converges but as expected for higher energies we need a higher precision to have a decent convergence and reliable results.

We can see see here that the method converges for higher precision. The numerical error tends to increase for shorter wavelengths, that is, for higher photon energy. So one approach is to check that the results converge for the specifications used in the system. [4]

2.2 The Parameters

In the simulation there are several parameters that we can change to find extreme values and resonances as well as other interesting features in the system. We can vary the nanowire length L, the nanowire diameter D and the period p of the square array. For the light, we can model different wavelengths and also the angles of the incoming light. Those options give us the possibility to explain, find and visualize characteristics of the nanosurface.

3 Results & Conclusion

3.1 Absorption vs wavelength and diameter of the wires

In figure 1 below we see the absorption in the InP nanowires against the wavelength and the diameter of the nanowires.

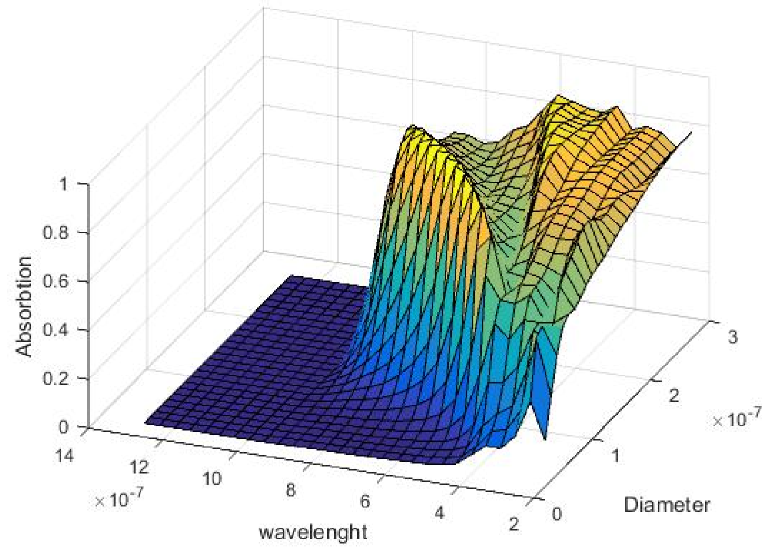

Figure 1: Plot of the absorption vs wavelength and diameter with a length of 900nm and period of 400nm

The first thing we see is that there is zero absorption for a wavelength bigger than 1000nm. This is because the band gap of InP, the material of the nanowires, correpsond to around 1000nm in wavelength. When the photon wavelength is above this value it can't be absorbed in the material anymore and no absorption will take place.

The next thing we see is a very high peak that follows a certain λ/D ratio, and for larger ratio's, the absorbtion drops quickly. The value of the ratio we determined to be around 3.3. The reason that there is less absorption for larger rations is because the waveform cannot resonate in the nanowire. Note that for smaller ratio's we see peaks that could be multiples of the γ/D ratio corresponding to higher harmonics. [2] The modes that are responsible for the absorption can be depicted as circular modes in the nanowire.

3.2 Absorption vs wavelength and period of the nanowires

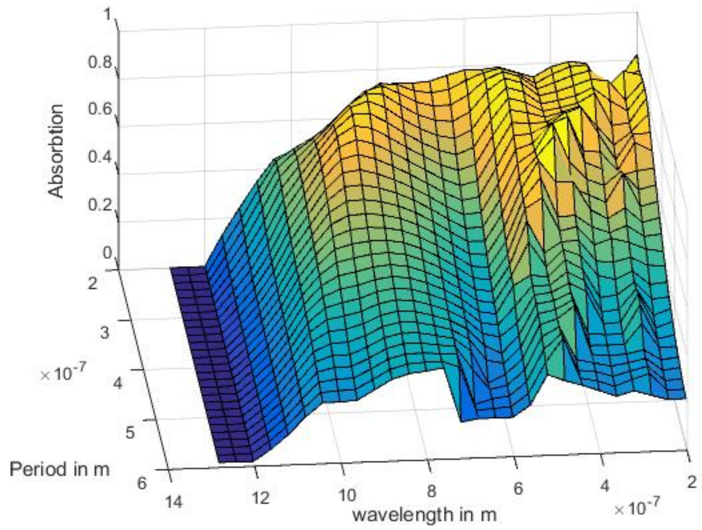

Figure 2: Plot of the absorption vs wavelength and period of the nanowire

The first thing we see is that the absorption goes to zero for wavelengths corresponding to lower energies than the band gap, as expected. As the period decrease we can see that the absorption increases. This is as expected because the concentration of nanowires increases and the light has to interact more with the wires and less light will actually reach the bottom.
We also see a peak for a P/λ ratio of 1 at the higher wavelengths (in the top right in figure 2), this probably has to do with the surface acting as a diffraction grating, and at $P = n * \lambda$ one of the higher order diffraction is at 90 degrees and gets absorbed by the nanowires instead of reflected from the nanowires.

3.3 Absorption vs diameter and period of the nano-wires

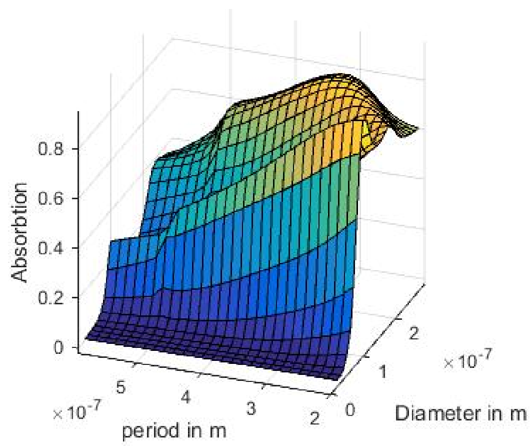

Figure 3: Plot of the absorption vs period and diameter of the nanowires with a light wavelength of 500nm

Here we can see a clear jump at p = 500nm because the wavelength used in the simulation is 500nm. For this normally incident light, for p ¡ 500 nm, only the specularly reflected light exists, whereas for p ¿ 500 nm, higher diffracted orders exist in reflection. In the presence of more reflection channels, we expect a higher relfectance, leding to lower absorption (that is, we expect more absorption when going to p ¡ 500 nm from p ¿ 500 nm, leading to the jump).

There is an optimum value for the diameter of the wires, if the wires become too thick, the light will reflect of the wires and if they become too thin the light won't interact with the wires and the light will reflect on the bottom. If the nanowire diameter will become $\sqrt{2}p$ then the surface will be completely flat and we can use the classical ray tracing optics again.

We can again see a peak through the whole plot for a diameter of a little bit more than 100nm, this corresponds to resonant absorbtion of the 500nm wavelength, in Figure 1 we can check that this value lies indeed on the peak there.

3.4 The reflection, transmission, and absorption versus wavelength at varies polar incidence angle

Figure 4 shows the absorption of light in the nanowire arrays for different wavelengths. The data for different angles is shown as seen in the legend.

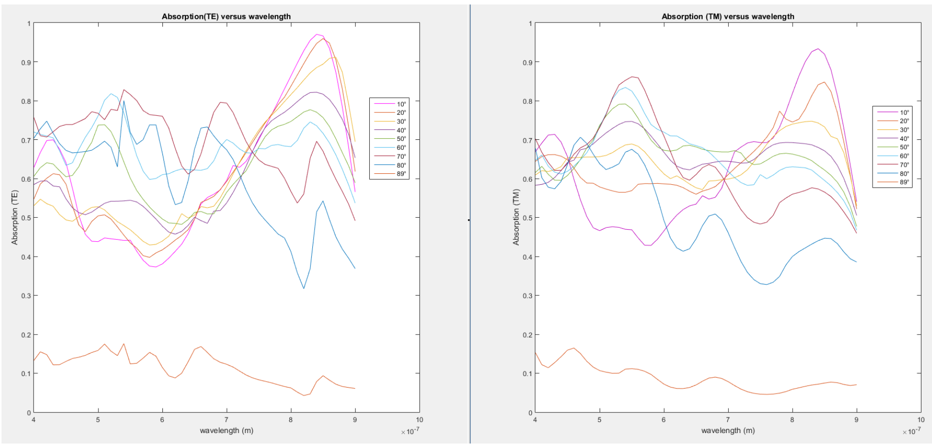

Figure 4: Plot of the absorption vs wavelength for different polar incidence angles with a nanowire length of 1 μm, a diameter of 180 nm, a period of 600nm and a azimuth incidence angle of 25 °

One can see that the polar incidence angle around 40°to 60°gives the best absorption. At 89°, the absorption is low. For higher angles, the light is reflected more from the nanowire top surface. This high reflectance when the polar angle goes towards 90^0 is a general characteristics of planar systems (even if the surface is corrugated, like here with nanowires). However, in most of devices the incidence angle of the light can be chosen by directing the device towards the light.

3.5 The length of nanowires dependence

The absorption, reflection, and transmission versus nanowire length are shown in figure 5.

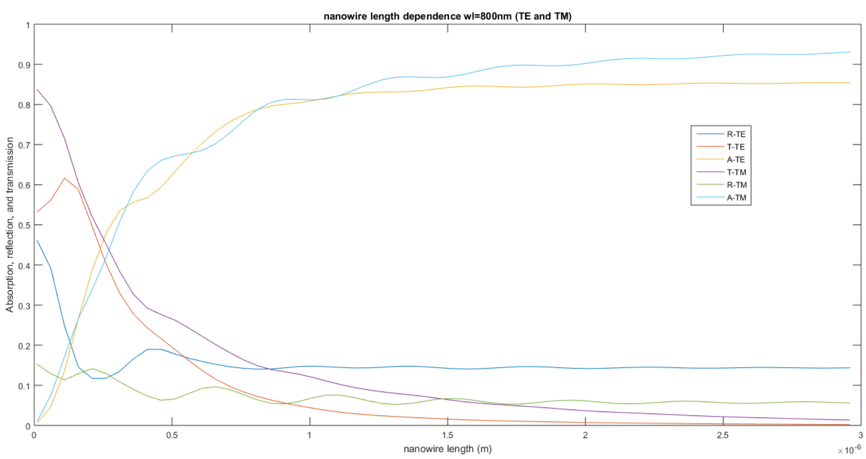

Figure 5: Plot of the absorption, reflection and transmission versus nanowire length for a wavelength of 150nm and 800nm. The diameter of nanowire is 400nm, period of the system is 600nm, azimuth angle is 25°and polar incidence angle is 50°

When the nano-wires are short we find a low absorption due to insufficient amount of absorbing material. When the length of the nano-wires is increased, we find an increase of the absorption because the light tends to interact with the nano-wires and gets absorbed.

Eventually, when the nanowires are long enough the absorption will asymptotically approach a value $1-R_{top}$ where R_{top} is the reflectance of the top surface of the nanowire array (typically, R_{top} decreases with decreasing D or increasing p).

Furthermore, we observe oscillation of the reflectance for small nano-wire length with roughly a constant period. This can be explained by an alternation of constructive and destructive interference in the system leading to an oscillatory behavior.

If we plot the wavelength dependence of the nanowire length as seen on figure 6, we can search for modes that travel vertically in the nanowire and will follow a line of constant wire-length/wavelength ratio and are coupled by $\lambda = n * \text{length}/2$. We can clearly see them in figure 6. Those peaks are all parallel and have the same distance between each other as expected.The 800nm peak corresponds again to the ratio for λ/D we found in the figure 1.

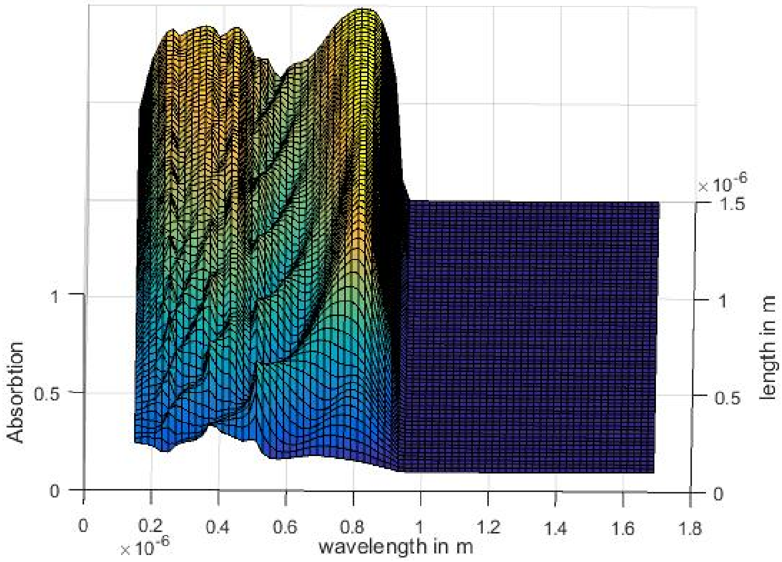

Figure 6: Plot of the absorption vas length and wavelength where period was 500nm and the diameter was 180nm

References

[1] K. Seo and al., *Multicolored Vertical Silicon Nanowires.* Nano Letters 11 1851 (2011)

[2] N.s Anttu *Geometrical optics, electrostatics, and nanophotonic resonances in absorbing nanowire arrays.* Opt. Lett. 38, 730 (2013).

[3] Ingvar Aberg and al., *A GaAs Nanowire Array Solar Cell With 15.3% Efficiency at 1 Sun.* IEEE. J. Photovolt. Online Early Access (2015).

[4] N. Anttu and H. Q. Xu *Scattering matrix method for optical excitation of surface plasmons in metal films with periodic arrays of subwavelength holes.* Phys Rec B83 165431 (2011)