# STUDY ON THE ABSORPTION AND SCATTERING EFFICIENCIES OF THE CADMIUM TELLURIDE NANOWIRE

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***ABSTRACT***

*The optical properties of cadmium telluride nanowires have been simulated using the Mie scattering coefficients. It is seen that the absorption efficiency shows multiple peaks along the spectrum due to leaky mode resonance. The nanowires showed strong polarization dependence in smaller radius. Higher angle of incidence showed a suppressing effect on lower valued peaks on absorption efficiency. Scattering efficiency showed peaks at visible spectrum from 30nm to 100nm. Transverse magnetic wave showed a more pronounced effect in scattering than transverse electric wave.*

***KEYWORDS***

*Cadmium Telluride, Nanowire Geometry, Scattering Efficiency, Absorption Efficiency , Mie Scattering Framework.*

## 1. INTRODUCTION

Cadmium telluride (CdTe) is a II-VI semiconductor material having a direct band gap of 1.44 eV at room temperature. Its high absorption coefficient has made it a material of wide interest and many applications [1]. In bulk form it's an ideal material for photovoltaic applications. Band gap engineering of CdTe has led to many applications in photo-detection and in other relevant fields [2]. CdTe quantum dot is a material of great importance in the current research field. Quantum confinement in such zero dimensional nano-materials offers a wide range of band gap tunability in the visible spectrum [3].

Like quantum dot nano-particles, CdTe nanowires have also received a lot of attention. A number of techniques have been developed to synthesize CdTe nanowires [4]. At first the solution based synthesis techniques were offered [5]. Then the self assembly of CdTe nanoparticles was also considered [4]. The recently discovered electro-deposition technique with template direction is the most efficient method for now because of the relative ease with which diameter is tuned [6]. While a lot of techniques have been used for synthesis of the nanowire, there have been few reports on the property studies of CdTe nanowires. An account of the electrical and optoelectronic properties is given in [7]. A detailed account of electronic structure and spectroscopy of nanowires is given in [8]. The advantage of nanowire geometry over ultra-thin geometry in absorption process of solar cells is discussed in [9].

In this article, we discuss the mechanism of scattering and absorption of light in CdTe nanowire under Mie scattering framework. So far we have seen a profound analysis of scattering and absorption phenomenon for Silicon and Germanium nanowires. The refractive index of the CdTe material is shown in Figure 1 [10]. The extinction coefficient of CdTe is small compared to Germanium within the visible spectrum. Again, in the visible spectrum, CdTe has an extinction coefficient higher than that of Silicon. This automatically translates into an intermediate absorption with strong resonance. These characteristics of the CdTe nanowires can be strongly used in plasmonics, photovoltaics and various in-situ characterization of CdTe nanowire itself.

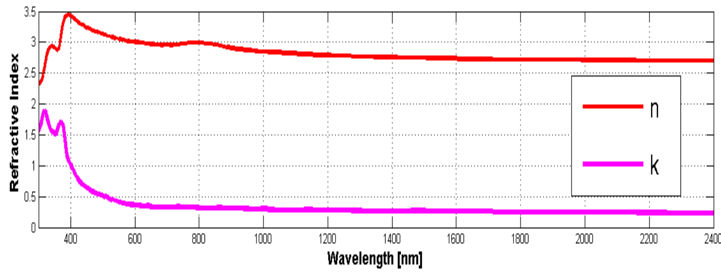



Figure1: Complex Refractive Index of the CdTe. Real part of refractive index is denoted by n and complex part is denoted by k.

## 2. DEVICE GEOMETRY AND SIMULATION METHOD

In this simulation study, we have used a nanowire structure as shown in Figure 2. The nanowire is placed in vacuum. It's assumed that the length of the nanowire is very long compared to the radius of the nanowire. The scalar plane wave incidence is determined assuming the nanowire is placed centred along the z-axis. Here, we have considered both transverse magnetic (TM) wave where the magnetic field is perpendicular to the nanowire axis and the (TE) wave have where the electric field is perpendicular to the nanowire axis as shown in Figure 2. Also, unpolarized wave have been considered.

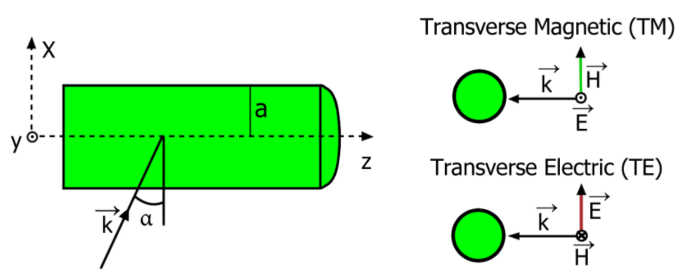



Figure 2: Schematic diagram of the nanowire and directions of transverse magnetic and electric fields.

The radius of the nanowire is given by a. The angle of incidence is denoted by α.In this article we simulate the absorption and scattering efficiencies of a nanowire made entirely of CdTe material. The absorption efficiency, $Q_{abs}$ , is described as the ratio of the absorption cross-section area and physical cross section area of the wire. The scattering efficiency, $Q_{sc}$ ,is similarly defined as the ratio of the scattering cross-section area and physical cross section area of the wire [11].

For simulation purposes the Mie scattering theory was used. A detailed analysis of Mie solution can be found in [11]. The Mie scattering solutions developed for circular cylinders were is used to solve for Mie coefficients of the systems. The simulator "Optical Properties of Single Coaxial Nanowires" available for free at NanoHub.org, has been used for simulation purposes [12]. The simulator uses following mechanism for calculating Mie coefficients.

First, the solutions for the 2D vector wave equation are determined in different spatial regions and the electromagnetic fields are expressed in terms of these solutions. Effectively, the vector wave equation is substituting the H field into the E field of Maxwell's equations. In 2D, these solutions take the form of a summation of Bessel functions, whose coefficients are determined from the boundary conditions. Then boundary conditions for continuity at interface are applied, which results in a system of linear equations. The problem can then be represented in a matrix form and the unknown Mie coefficients can be computed. Using the calculated Mie coefficients, the total scattering, absorption and extinction efficiency can be determined. A complete mathematical account of Mie scattering in this process can be found in [12].

## 3. STUDY ON THE ABSORPTION EFFICIENCY

At first, the absorption mechanism of CdTe nanowires is studied. Bulk CdTe has a direct band-gap of about 1.529 eV at 300K. An interesting phenomenon occurs at nanostructured CdTe. The band gap becomes tunable with respect to the dimension of the body while maintaining its direct nature. Such band gap engineering is also prominent from studies of CdTe quantum dots.

Figure 3 shows the spectral measurement of $Q_{abs}$ for nanowire radius 20nm, 50nm, 80 nm and 100 nm respectively for perpendicular illumination of un-polarized light. For every data we see that there are multiple peaks in the wavelength range. This is quite different from the absorption nature of bulk CdTe. The reason behind this can be explained by leaky mode resonance. A similar calculation of the leaky mode resonances in similar Germanium nanowire is given in [13].

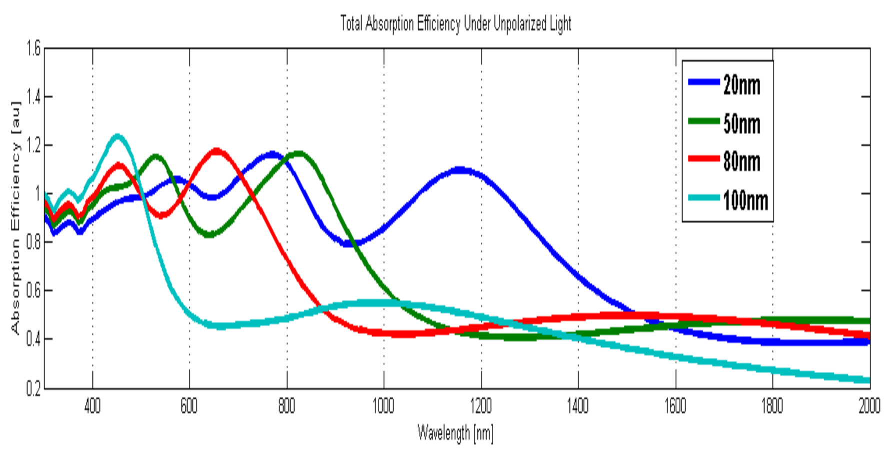
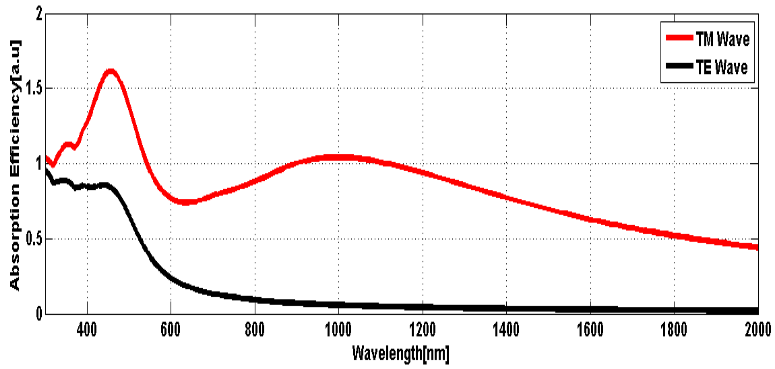
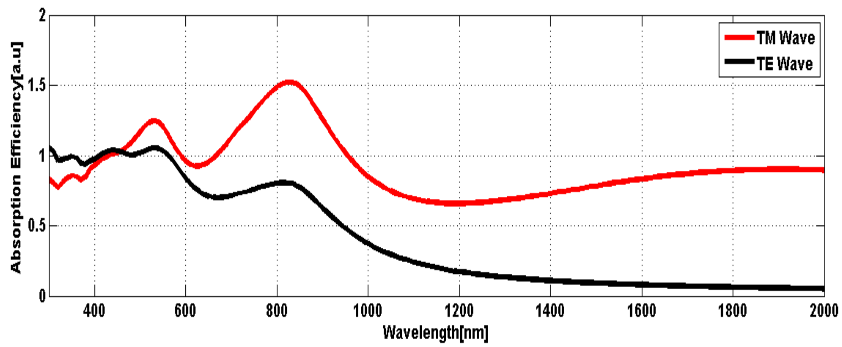



Figure 3: Multiple Peaks resulting from leaky mode resonances for various nanowire radii.

Figure 4(a) and Figure 4(b) shows the effect of TM mode and TE mode on the absorption characteristics of CdTe nanowires for nanowire radius 50nm and 100nm respectively. It's evident that transverse magnetic mode leads to a lot more absorption than transverse electric mode.




(a)




(b)

Figure 4: Effect of Transverse Magnetic and Transverse Electric wave on absorption Efficiency for (a) 50nm and (b) 100 nm.

However, in Figure 5, the TE/TM absorption efficiency ratio was plotted as a function of radius for 600nm wavelength. It predicts that for a given wavelength the ratio is very high for small radius nanowires. But, decreases rapidly as radius increases and eventually becomes steady. This is quite obvious for leaky mode resonance mechanism. When the diameter is small, only fundamental and lower modes can be supported by the nanowire. This in return results in strong polarization dependence. Because of heavy degeneracy of transverse magnetic and electric modes, the polarization dependence falls sharply at nanowires with higher radius.

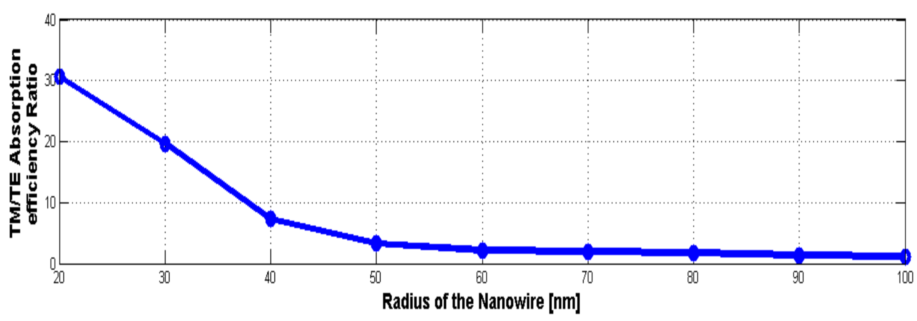



Figure 5: TM/TE absorption efficiency ratio versus radius of the nanowire for 600nm wavelength.

Figure 6 shows a study of the absorption efficiency for angle of incidence of 0° (indigo), 20° (red), 45° (green) and 60° (blue) respectively with unpolarized light at core radius 50nm.While the major peak of absorption remains almost the same, changing the angle of incidence causes other peaks to subsidized. This is because of the fact when the incident angle is changed instead of TE and TM modes hybrid modes are induced in the nanowire.

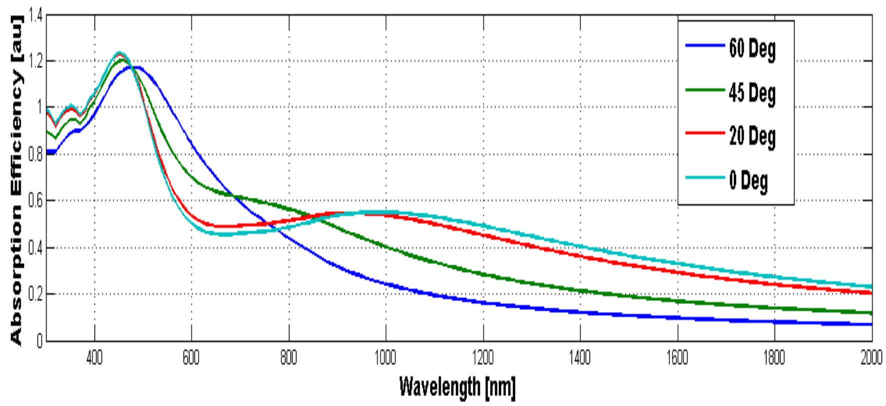



Figure 6: Variation of Absorption efficiency with angle of incidence.

## 4. STUDY ON THE SCATTERING EFFICIENCY

Scattering from nanowires are directly proportional to the illumination and scattering efficiency $Q_{sca}$, of that nanowire. Figure 7 shows the relation between the diameters of the core with scattering efficiency for TM light with normal incidence to the nanowire axis. Interesting behaviour of scattering is seen from diameter 30nm to 100nm as shown in Figure 7.

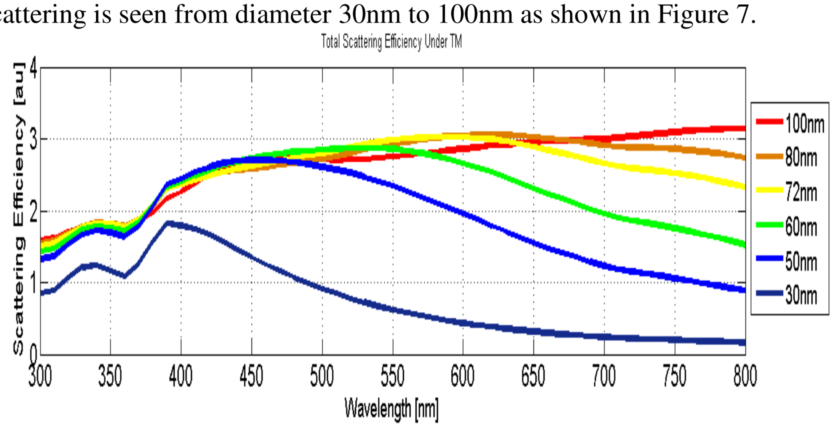



Figure 7: Effect of Radius on Scattering Efficiency for various diameters of the nanowires under Transverse magnetic field for perpendicular Illumination.

For diameter 30nm we see a sharp peak at 390nm. This implies a sharp scattering of violet light. As the diameter of the nanowire is increased, scattering efficiency also increases. But, more importantly, peak shifts with increase in diameter. At diameter of 50nm, we see peak at blue region of visible spectrum with higher scattering efficiency than before. Similarly, at diameter 60nm, 72 nm and 80 nm we see the peak at green, yellow and orange region of visible spectrum. At 100nm we see large scattering efficiency in the red region. These are very common diameters for CdTe nanowires. So, we can use this knowledge in the growth of the CdTe nanowires.
Figure 8, 9 and 10 illustrates the complete relation of scattering efficiency with the diameter of the nanowire and the incident wavelength for unpolarized light, transverse magnetic wave and transverse electric wave respectively. It's evident that the response to the transverse magnetic

wave is profound when compared to the transverse electric wave. From both unpolarized light and TM polarized light, it can be seen that scattering efficiency is not that prominent for any diameter before wavelength is 370nm. Scattering efficiency becomes prominent after that and shows a variable relationship with the diameter.

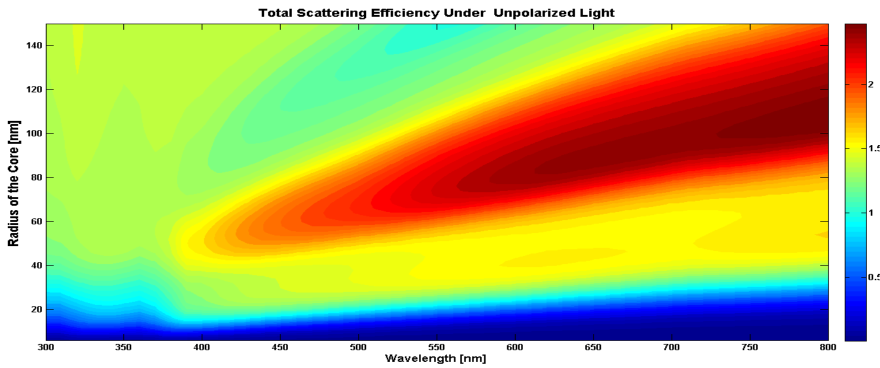



Figure 8: Total scattering efficiency for Un-polarized light for various wavelength and radius of the core.

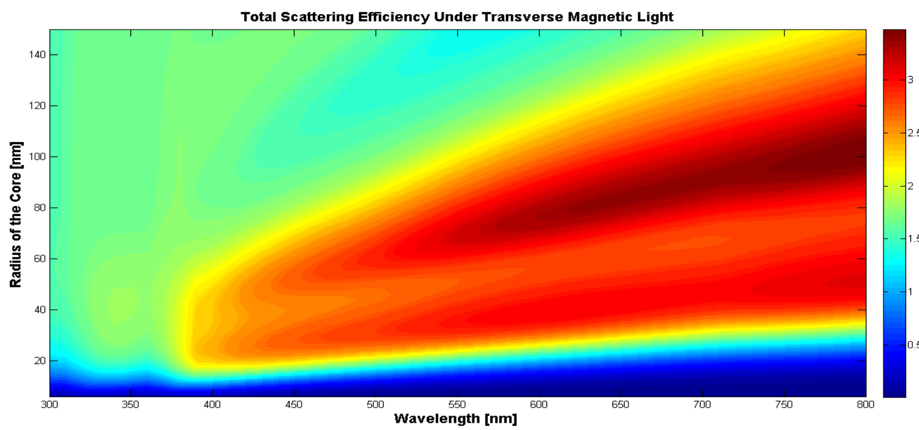



Figure 9: Total scattering efficiency for Transverse Magnetic Wave for various wavelength and radius of the core.

## 3. CONCLUSIONS

In this paper, we have studied the optical scattering and absorption properties of cadmium telluride nanowires. Scattering and absorption efficiencies were simulated using the Mie scattering framework. The effects of diameter of the nanowire, polarization and angle of incidence on absorption efficiency were thoroughly discussed. It's clear that leaky mode resonance plays a vital role in the absorption mechanism. The effect of diameter on scattering

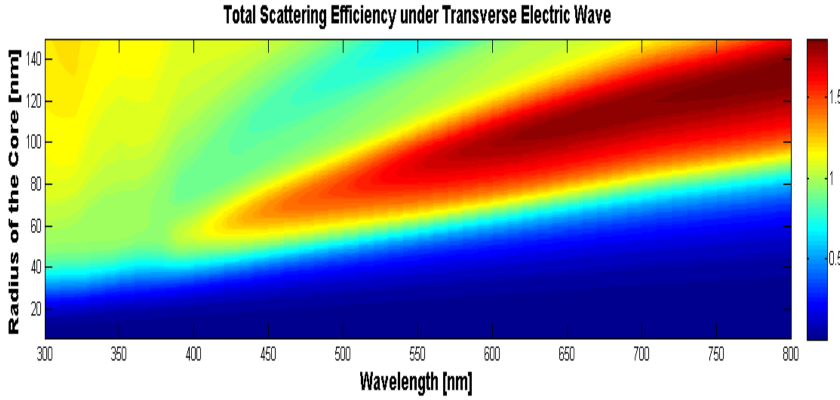



Figure 10: Total scattering efficiency for Transverse Electric Wave for various wavelength and radius of the core.

efficiency was also simulated separately for unpolarized, TM and TE wave. Scattering efficiency showed sharp peaks at visible spectrum. And peaks changed with the change of diameter. This opens the possibility of in-situ control of diameter growth of CdTe nanowire.

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