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# Computational Investigations on CZTS Thin-Film Layers Adopting Grating Structures

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***Abstract***

*In the past few years, Copper zinc tin sulfide ($Cu_2ZnSnS_4$, CZTS) has attracted significant attention as a next-generation absorber material for the production of thin-film solar cells on large scales due to the high natural abundance of all constituents, the tuneable direct bandgap energy ranging from 1.0 to 1.5 eV, and significant absorption coefficient. Copper zinc tin sulfide (CZTS) is a promising material for use at a low cost.*

*In this work, simulations were performed on CZTS thin-film solar cell (TFSC) using the FDTD method; the Continuous Gaussian Wave of 1.55 wavelength light incident input applied. Three different methods performed in simulations. Results indicated that the heat absorption efficiency of the solar cell increased when grating structures are designed to be on the surface of the solar cells. The efficiency was increased by 17.64%. It observed that when the grating period "k" is varied, the absorption efficiency is also varied; higher the grating period lower the absorption efficiency and vice versa. The weighted reflectance of the CZTS TFSCs having grating structure reduced to 1% of the value. It also observed that maximum absorption efficiency occurs at lower wavelengths of 480nm to 800nm. When the wavelength increased beyond, then there is no noticeable change in its effectiveness.*

**Keywords—***CZTS, TFSC, FDTD method, Adopting Grating Structures, solar cell*

## I. INTRODUCTION

In optoelectronic devices, Anti-reflection coatings (ARCs) play a vital role. ARC has an excellent ability to minimize Fresnel reflection loss while the interaction of light and semiconductor material [1]-[7]. Traditionally single-layer or multilayer stacks of the film used for ARCs during some close spectra of incident wavelengths and angles, essentially silicon nitride or silicon dioxide [8], [9]. Though, both extend over definite drawbacks. Before mentioned being substance choice, thermic mismatch induced lamination, and precise thickness control [10]. The origin of these anti-reflective properties emerged from a continuous gradient of the refraction index between air and the corneal surface and was suggested as the ultimate solution to suppress light reflection in the entire solar radiation spectrum. In addition to that, when the grating period is almost like the value of light incident wavelength, then light wave can be resonating and can be reflected inside the structure, which can because of the resonant reflection in the device [11].

Moth-Eye Structure is well known as the anti-reflective surface structure, used in different works. The FDTD is used to perform simulations on moth-eye nanostructures, decreasing reflectance and improving the solar cell's efficiency. This antireflection property of moth-eye structure has many applications in sensors, detectors, military and solar energy [12]. Similarly, in another work, it is concluded that the anti-reflective property of moth-eye structure can improve the relative power conversion efficiency (PCE) of a solar cell, having a reflectance index of 3% and a wavelength range 570 to 950nm [13].

However, CZTS TFSCs nowadays consider the second generation of solar cell technology. The main advantage which this technology provides in this decade is the cost reduction over the other wafer-based solar technologies and the abundance of components available in the earth crust, which are essential for CZTS TFSCs. Currently, there are three leading thin-film solar technologies that are ruling the market of solar technology are amorphous silicon (a-Si), Cadmium Telluride (CdTe), and CIGS. Among these three, CIGS has an efficiency of 20% on lab-scale cells, while the other Cadmium Telluride holds a high share in the market. The main hindrance to CIGS is the scarcity of Indium and Gallium on the earth's crust and the environment's problem. To reduce the cost of unit generation per watt and increase solar cells' efficiency, Multi-junction solar cells are the best choice because they work by capturing the high energy photon and extracting the energy from it as higher as possible, and then the second junction occupies the lower energy photon. The first layer in such type of multilayer junction cells can be an organic semiconductor having a large bandgap, and the second layer can be an inorganic semiconductor, which is the same as CZTS TFSCs. The theoretical efficiency of such solar cells can be as high as 42% [14]. Nowadays, the practical efficiency record of CZTS TFSCs has reached 9-11%.

After the study of Katagiri et al., which started early in the 80s and 90s, CZTS TFSCs has attracted attention from all around the world, and there is quite an improvement in efficiency since then. QijieGuo et al. tuned the crystals of CZTS and achieved an efficiency of 7.2% under AM 1.5. Also, light soaking was produced by this work [15]. Hossain et al. using numerical analysis, replaced the Cds by the ZnO, ZnS, ZnSe, and InS as a potential buffer layer to the CZTS [16]. Kazuo Jimbo et al., in this research author obtained the 5.74% efficiency of CZTS using the Inductively Coupled Plasma Spectroscopy (ICPS) technique. By this technique material of CZTS was analyzed [17]. Tanka Raj et al.studied CZTS chemical bath deposition was introduced for deposition and obtained an estimated bandgap (1.48 ~ 1.51 eV) for CZTS [18]. Vanalakar et al. proposed the CZTS and prepared it as a target for PLD Deposition, and authors also discussed the solar cell performance of CZTS thin-film solar cell by the survey of pulsed laser CZTS thin films [19].

This work is also carried out to determine the absorption efficiency of CZTS TFSCs using Opti-FDTD simulation software. Three different types of simulations are performed, having three different designing techniques. Firstly, the multilayer structure was designed by using the PBG Photonic Band-Gap Crystal technique to provide the fundamental periodic structure of grating material with equally spaced grating and period, and since the Fibre Profile Channel structure was considered, that is why the structure is round. The second design is done by Computer-Aided Design Technique using vertical input source which is an easy way to design and in the third method instead of simple input source TFSF (Total Field Scattering Field) input source choose, and results and discussions explained in detail.

## II. COMPUTATIONAL DETAILS

In this work, we only include the FDTD method in our simulations since Opti-FDTD software utilized this numerical technique. FDTD techniques have appeared as an essential way to solve many scientific and engineering problems explaining electromagnetic waves interference with materials structures. It switches Maxwell equations into the time domain and spatial domain equations from differential equations, which determine the values of the electric and magnetic field of the light at a discrete space and specific time [20]. Following the flow chart is shown in Fig. 1 describes the complete methodology of Opti-FDTD.

The layer thickness for CZTS TFSCs used for simulation purposes is shown in Fig. 2 and the maximum values of thickness are taken in design for CZTS in Opti-FDTD.

Glass Substrate thickness varies in different designs; in our case, the glass substrate thickness is 2. The grating period "K" is chosen as 0.3, grating spacing "d" is 0.1, and the grating structure's width is 0.1. Since in the last chapter, we discussed the effect of grating design briefly along with the simulation results, that is why it is always essential to select wisely the shape of the grating structure. In this case, linear taper gratings are used, having a starting thickness of 0.5 and an end thickness of 0.15. In the simulation process, the Continuous Gaussian Wave input wave applied in all three instances having a wavelength of 1.55 with a normal incident angle. The boundary conditions selected as Periodic Boundary Conditions (PBC) in the x-direction and Perfect Matching Layer (PML) boundary conditions are in the z-direction, which helps absorb the incident going away from the design. As previously described, to get accurate simulation results, the mesh size must be 1/10 of input wavelength; that is why the mesh size selected as 0.15. 2D simulations are performed, which are fast and reliable and acquire less memory and time consumptions as compared to 3D simulation.

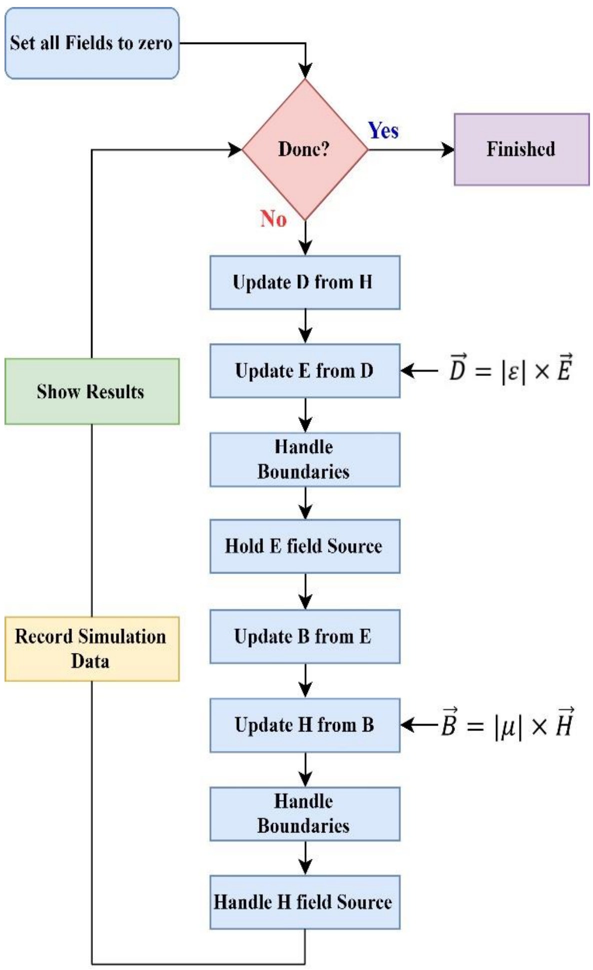



**Fig 1: Flow chart for the complete process of the FDTD method**

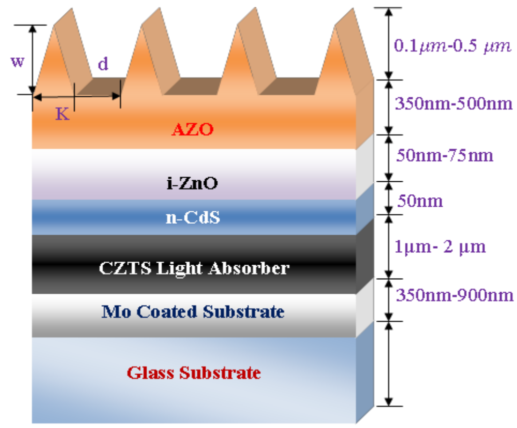



**Fig 2: CZTS TFSC layer structure**

## III. RESULTS AND DISCUSSION

### *A. Multilayer structure design by photonic bandgap structure method*

Diagram obtained by using this method is shown in Fig. 3, which shows the Simulation window, the 3D model layout of CZTS TFSCs, and the refractive index distribution of the layers.

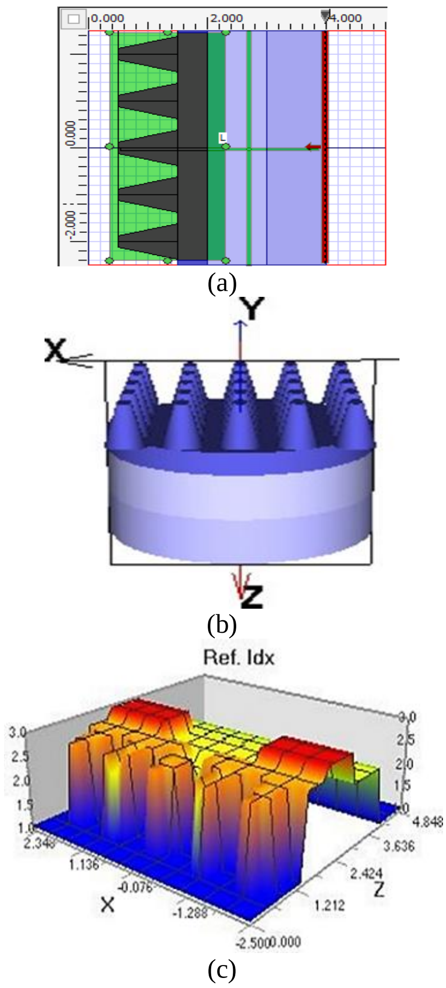



**Fig 3: (a) Simulation window showing CZTS layers along with grating, (b) 3D Model layout of CZTS TFSCs, and (c) Refractive index distribution of multilayer structure**

#### *a) Simulation results of CZTS by PBG method:*

To obtain the heating absorption plot for the design, the simulation process utilized is the photonic bandgap crystal lattice structure method. That is the reason for using this technique to design our multilayer structure. After running a 2D simulation, the results obtained are presented in Fig. 4.

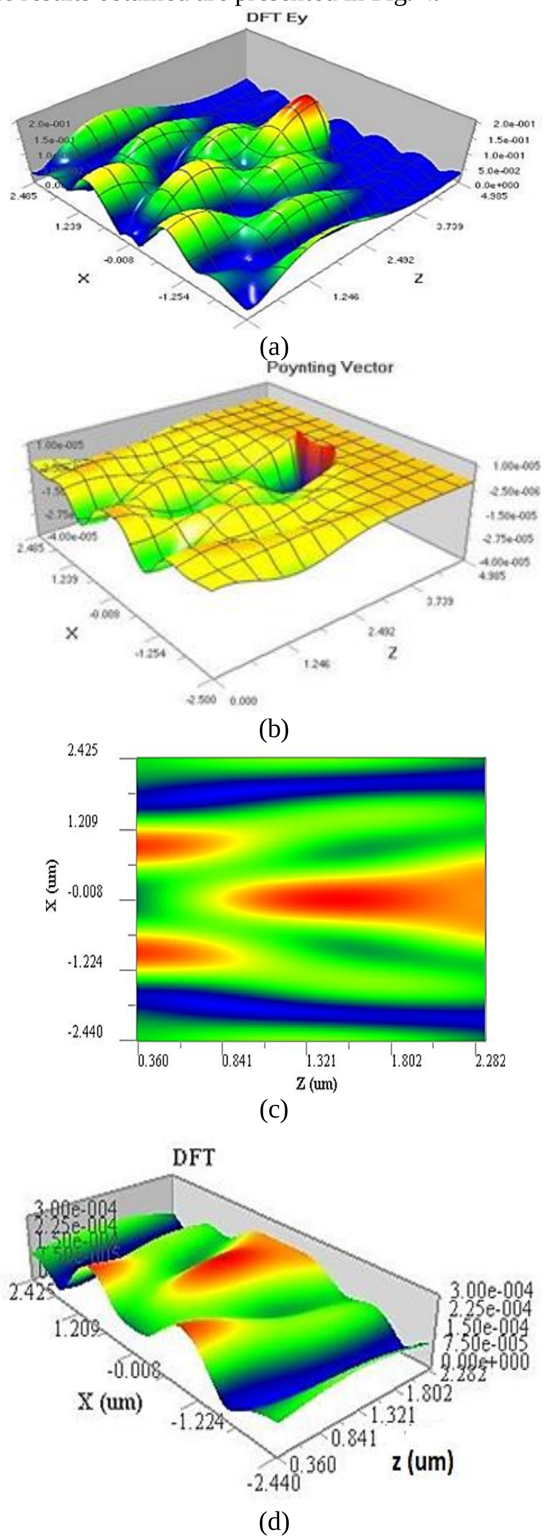
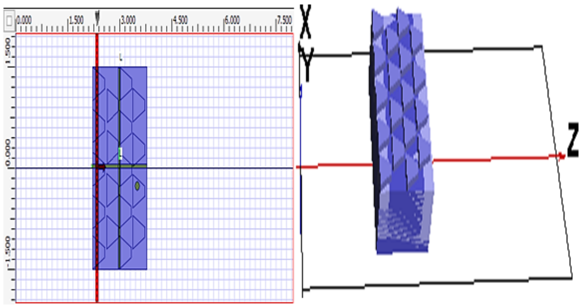


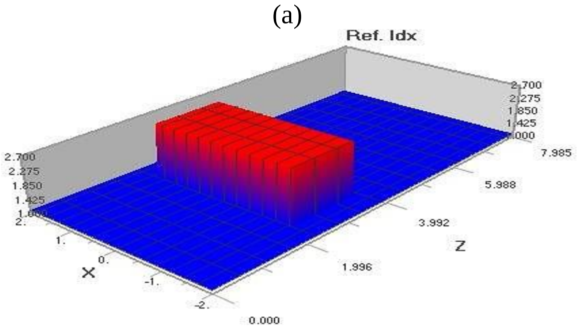

**Fig 4: (a) 3D Plots of DFT Ey and (b) Poynting vector (c) Heat absorption image plot (d) Heat absorption height plot**

### B. CZTS TFSCs design using the CAD design method

The design obtained by such an approach is in Fig. 5.




(a)




(b)

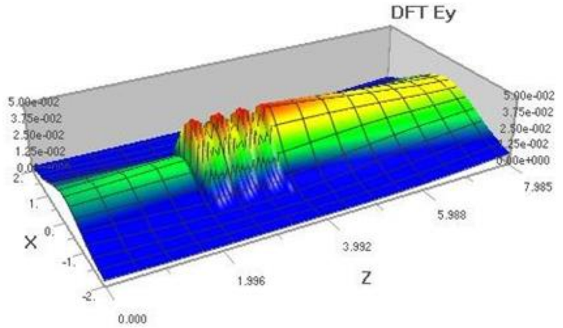
**Fig 5: (a) Simulation window showing CZTS layers along with gratings and 3D model layout of CZTS TFSCs and (b) Refractive index distribution of multilayer structure**

*a) Simulation results for the CAD environment design method:*

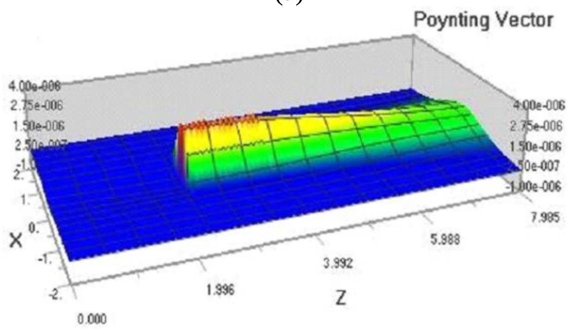
The grating period and spacing are the same as in the first design method, only the difference is that in the last case, 5 periodic gratings were used in each row, while in this case in the first row 5 periodic gratings are used, and in the second row 4 periodic gratings are used, and so on. The simulation results obtained are present in Fig. 6.

*b) Discussion for results:*

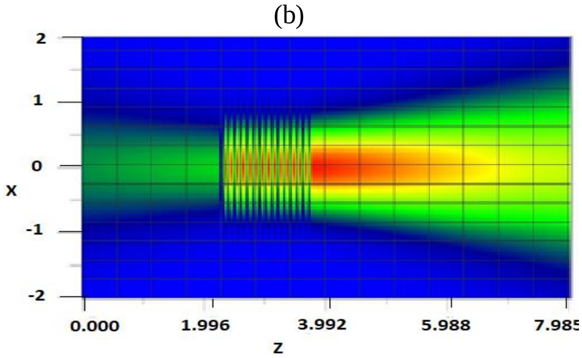
If we correlate results amidst the past simulations, then there is a small difference in field distribution and heat absorption in the device. In this case, since the gratings are on the top of the CZTS cell and vertical input plane applied, then the firstly the incident wave is absorbed by the grating structures as shown in Fig. 6(c), and then it is traveled through the multilayer structures. While the energy absorbed is higher at the surface because the AZO grating structure acquires higher energy photons first, and then they move through the device, as shown by Poynting Vector in Fig. 6(d). In the previous simulation process, there was no light reflected beyond the point of the input source, but if we notice carefully, the color Palette graph of DFT Ey in Fig. 6(c), there is a small amount of light incident wave reflected from the point of input source position. Even these grating structures provide the Anti Reflection effect at their best, but still, they have a reflection of 9.9 %.



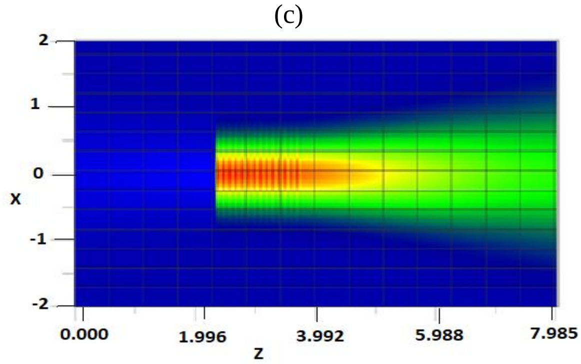

(a)




(b)




(c)

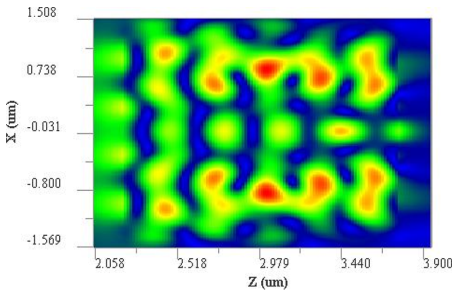



(d)

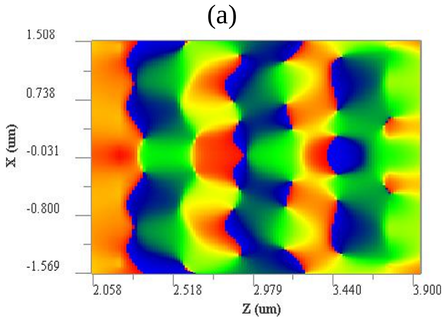
**Fig 6: (a) DFT Ey, (b) Poynting vector (c) DFT Ey in color palette shape, and (d) Poynting vector in color palette shape**

### C. Heat absorption amplitude and phase plots

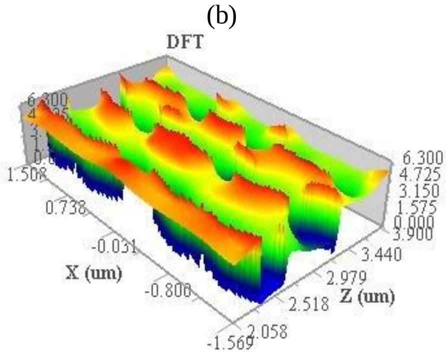
In Fig. 7, Phase distribution plots clearly show the direction of heat absorbed inside the layers from the grating structure then diffracted inside the layers. That is the primary purpose of diffraction gratings, which diffract and divide the light in such a direction so that the maximum amount of energy should be extracted from the light incident, and high energy photons should be trapped easily in the device structure.



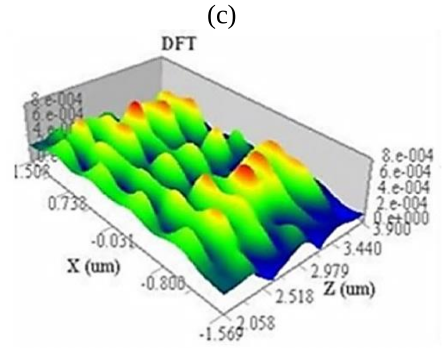

(a)




(b)




(c)




(d)

**Fig 7: TFSF TE simulation results showing 3D Plots of (a) Heat absorption image amplitude plot (b) Heat absorption image phase plot (c) DFT Heat absorption height amplitude plot (d) Heat absorption height phase plot**

## *D. The power spectrum of CZTS TFSC*

The Spectrum plot of CZTS TFSC produced after the simulation is given in Fig. 8. This power plot spectrum illustrates that when at a smaller wavelength, there is higher photon absorption. Hence there is more heat transfer through the CZTS TFSC. From Fig. 8 given below, it is shown that the Radiation Transfer in the CZTS TFSCs will have higher values at the wavelength between 0.5 to 4 wavelength periods.

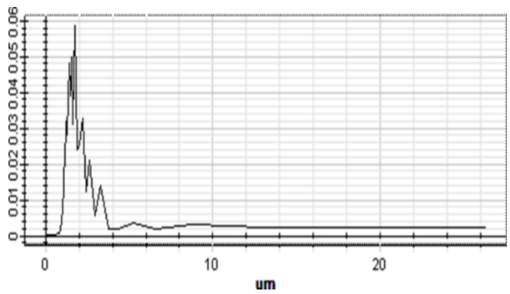



**Fig 8: Spectrum analyses of CZTS TFSCs**

## *E. Scattered/Reflected field graph*

The reflectance of the device is given in Fig. 9. The reflectance plot obtained here has the highest value of 8%. The variation in reflectance depends upon the design method of CZTS and the layer structure of CZTS cells.

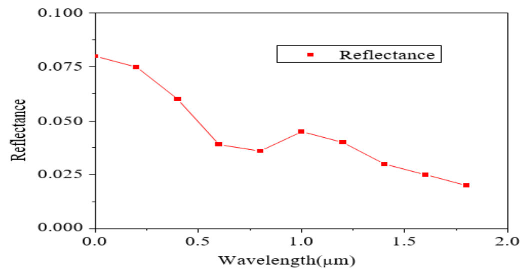



**Fig 9: Reflectance of CZTS TFSCs vs. wavelength**

## *F. Absorption efficiency of CZTS TFSCs*

Table I given below provides the values of Absorptance efficiency at each wavelength for the grating period "K". The grating period ranges from 0.3 to 0.4, 0.5, and 0.6. The wavelength was from 0.5 to 1.

**TABLE I**
**Absorptance of CZTS TFSC at grating period "k"**

| Grating Period "K"/Wavelength | 0.3 | 0.4 | 0.5 | 0.6 |
|---|---|---|---|---|
| 0.5 | 0.041 | 0.05 | 0.41 | 0.045 |
| 0.6 | 0.47 | 0.53 | 0.45 | 0.37 |
| 0.7 | 0.51 | 0.49 | 0.47 | 0.39 |
| 0.8 | 0.53 | 0.52 | 0.41 | 0.42 |
| 0.9 | 0.55 | 0.56 | 0.49 | 0.46 |
| 1.0 | 0.62 | 0.60 | 0.54 | 0.5 |

The plot generated by the values present in Table I is in Fig. 10, which differentiates the fact that if the grating period is lower, it increases the absorption efficiency of the solar cell.

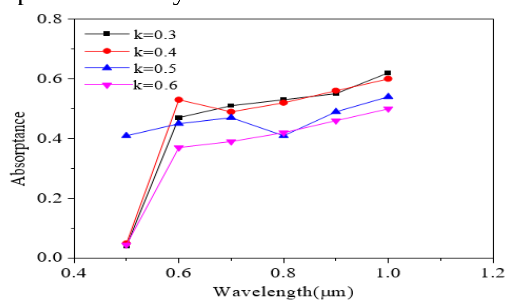



**Fig 10: Absorptance efficiency of CZTS TFSCs vs. wavelength**

## IV. CONCLUSIONS

Adopting the finite difference time domain (FDTD) method, the thermal radiative properties (i.e., absorption, reflectance, and transmittance) and the power conversion parameters for CZTS solar cells with grating structures were studied in detail. Obtained results indicated that the light absorption efficiency of the CZTS solar cell could be enhanced using AZO anti-reflective gratings on its surface. Further, light to power conversion efficiency depends on the grating period; if the period is kept smaller, higher power can be achieved. It is also observed that if AZO tapered gratings are used on the surface of the CZTS TFSC, the power absorption efficiency is moving to a higher value at the lower wavelengths in the range of 0.45to 1.0 arbitrary units (a.u). In this study, the maximum efficiency was obtained as16.2% having a grating period of 100nm. Since absorption and reflectivity have inverse relation, thus increased absorption defines reduced reflectivity. In terms of interlayer transmittance, the CZTS absorber layer increases the interlayer transmittance, thus allowing maximum light absorption inside the solar cells. It can be concluded from our study that grating structures can easily enhance the power efficiency of CZTS solar, thus allowing a unique way to modify the thermal radiative properties of CZTS cells, making them functional for renewable energy applications.

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