Enhancing the Opto-electronic Performance of Cadmium Telluride Thin-film Solar Cells Using Nanocone-shaped Surface Texturing

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***Abstract*—The domination of Cadmium Telluride (CdTe) in the thin-film solar cells (TFSCs) market is expected to continue in the future and overtake other types of TFSCs. This is due to the near-optimal bandgap energy, higher absorption coefficient, and low production cost of CdTe TFSCs. However, the efficiency of CdTe TFSCs needs to be significantly improved by addressing the optical losses taking place within the solar cell. Surface reflective loss accounts for a significant portion of these optical energy losses. This study uses finite-difference time-domain (FDTD) numerical method to investigate the effect of nanocone-shaped texturing of the Cadmium Sulfide (CdS) window layer of CdTe TFSCs on the opto-electronic performance of such solar cells. The study aims to optimize the nanocone morphology, solar cell performance parameters such as short circuit current density (J_{sc}), open-circuit voltage (V_{oc}), efficiency and others have been analyzed. The results suggest 13.91% increase in J_{sc} and 14.13% efficiency enhancement can be achieved for nanocone texture having a diameter, height, and pitch of 600 nm, 400 nm, and 75 nm, respectively. Further comparison with plasmonic metal nanoparticle-incorporated CdTe TFSCs indicates surface texturing to be a preferable choice over plasmonic metal nanoparticles for efficient light trapping/absorption in TFSCs.**

***Index Terms*—Cadmium Telluride, Thin-film solar cell, Finite-difference time-domain, FDTD, Nanocone, Nanostructure, Surface texture, Absorption, Reflection, Renewable energy.**

I. Introduction

The main function of a solar cell is to harness the power of the sun, yet most present-day solar cells lack the efficiency to do so on a commercial scale. Being the most common source of renewable energy generation, the lack of efficient conversion of solar energy is what enables fossil fuels to still dominate in energy market today. Although c-Si holds the lion's share of the entire solar cell market, the demand for thin film solar cells (TFSCs) is on the rise due to its thin absorber layer and high photo-conversion efficiency. Additionally, because c-Si is at least 350 times thicker than a TFSC, the cost of fabrication is relatively low for TFSCs as less material is needed [1]. Among all types of inorganic TFSCs, CdTe tops the list due to the fact that it has a near-optimal band gap energy (1.44 eV), allowing it to potentially reach the maximum efficiency possible by a single junction solar cell based on the Shockley-Queisser limit [2]. Furthermore, CdTe is a direct bandgap energy material and also has a higher absorption coefficient of 10^4 cm^{-1}, empowering it to absorb 92% of incident visible light having only just a 1 μm thick absorber layer [2]. The potential use of CdTe TFSCs includes smartphones, smart watches and other wearable gadgets, automobiles, drones, building-integrated windows, etc. Despite having the potential to achieve higher efficiency, several types of optical losses contribute to limiting the photon absorption within the absorber layer of the TFSCs. One of the most dominant optical losses is the reflection of light at the top surface of the solar cell. This reflection, also known as Fresnel reflection, is part of incident light energy that is reflected back from the interface of two propagation media having different refractive indices [3]. The Fresnel reflection coefficient depends upon the refractive index of the of two adjacent media through which light is passing (e.g., air and CdS-CdTe) as well as the angle of incidence of the incident light [3]. In a theoretical study, it has been found that reflective loss accounts for approximately 9% decrease in short circuit current density (J_{sc}) for CdTe solar cells [4]. To overcome the reflective losses at the front surface and to increase the chances of photon absorption for electron-hole pair generation, several techniques have been used over the last two decades among different types of solar cells [5] [6] [7]. Texturing the front surface of the solar cell is a common technique used to reduce reflection in many devices, yet it is not very widely used in TFSCs applications. Surface texture can help to trap the light within the absorber layer of the solar cell while functioning as an anti-reflective layer at the same time [8]. Furthermore, periodic surface texture enhances the optical path length into the absorber layer resulting in the optical path length increasing by several-fold over the physical thickness [9] [10]. The morphological features (height, width, pitch, etc.) of the surface texture cannot be greater than the wavelength of the incident light in order to harness the desirable light absorption characteristics [11]. Because the TFSCs' thickness is limited to nanometers to a few micrometers range, subwavelength surface textures (texture morphology scale is less than the wavelength of the incident light) are more desired in the case of TFSCs [11]. Subwavelength-sized surface texture works as an effective medium of gradually varying refractive index between two mediums having different refractive indices in contrast to the abrupt change of refractive index in the case of a flat surface [8]. According to the Fresnel reflection equation, the amount of light reflected from the interface between materials of two different refractive indices is directly proportional to the difference in refractive index of those materials [3]. A gradually varying refractive index due to sub-wavelength texture will therefore decrease the reflection and thereby increase the possibility of transmission of the incident light into the substrate [12]. Among different subwavelength texture structures, upright cone-shaped textures have previously shown superior enhancement in light absorption both in experiments and simulations [13]. Chemical Vapor Deposition (CVD), Reactive Ion Etching (RIE), and Ion Beam Sputtering (IBS) are several fabrication techniques used to texture the top surface of the TFSC by providing good control over the morphology of the texture and shape [14] [15] [16]. This computational study involves using nanocone-shaped textures on the window layer (CdS) of CdTe TFSCs and optimizing the morphology of the nanocone texture to achieve higher efficiency by reducing the surface reflection of light. This study will therefore help decarbonization by contributing to efficient renewable energy production and be a sustainable technology.

II. Material and Methods

A. Simulation Setup

Commercially available software FDTD Solutions and CHARGE from Ansys Lumerical Inc. have been used to carry out the simulations in this study. At first, the optical simulation was done in FDTD Solutions and later unfolded data was imported into CHARGE for the electrical simulation. Fig. 1 shows the three-dimensional (3D) illustration of the FDTD simulation setup. The top layer consists of a CdS window layer having a thickness of 100 nm along with an array of nanocone textured entities. This is followed by the absorber layer of CdTe with a thickness of 1500 nm. The bottom metal contact is designed with a 100 nm thick silver (Ag) layer thus making it work as a back reflector. Transparent Conductive Oxide (TCO) layer has been omitted since optical simulation does not require top contact and to reduce design

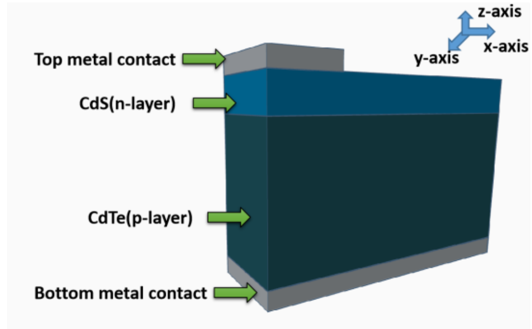

Fig. 2: CHARGE simulation setup conducting electrical analysis for CdS nanocone textured surface of CdTe TFSCs

complexity. The FDTD simulation region consists of only one nanocone as the light-matter interaction of adjacent nanocones was replicated by using the periodic boundary conditions. A plane wave was taken as a light source following the Standard Test Condition (STC) of AM 1.5G solar spectrum and 1000 W/m^2 light intensity. The wavelength range was set from 400 nm to 1100 nm according to the standard followed to test the solar cells opto-electronic performance parameters. Fig. 2 shows the 3D schematic of the CHARGE simulation setup. The thickness of CdS and CdTe remains the same as in the FDTD simulations. The CdS layer served the role of a window layer and was n-doped (doping concentration of 10^{14} cm^{-3}) while the CdTe layer served the role as the absorber layer and was p-doped (doping concentration of 10^{16} cm^{-3}). Finally, Fig. 3. demonstrates the nanocone morphological parameters that have been varied for the optimization of the surface texture to provide an enhancement of efficiency in CdTe TFSCs. The fundamental morphological parameters of interest are: diameter (D), height (H), and side-to-side spacing or pitch (P).

B. Numerical Background

All simulations were run in the wavelength range spanning from 400 nm to 1100 nm. Short circuit current density (J_{sc}) which is dependent upon the incident radiation's wavelength and power absorbed by the solar cell substrate was calculated using equations used in previous studies. Electrical simulations

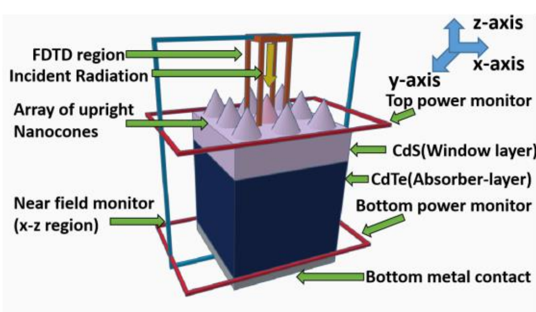

Fig. 1: FDTD simulation setup conducting optical analysis for CdS nanocone textured surface of CdTe TFSCs

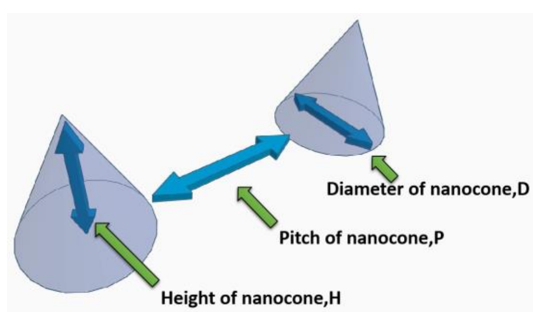

Fig. 3: Fundamental morphological parameters of the nanocone texture array investigated in this study

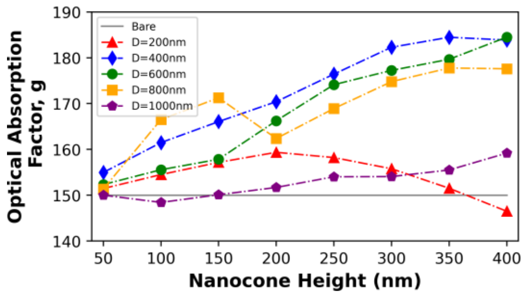

Fig. 4: Graphical representation of the optical absorption factor for nanocone texture ranged 50-400 nm in height and 200-1000 nm in diameter.

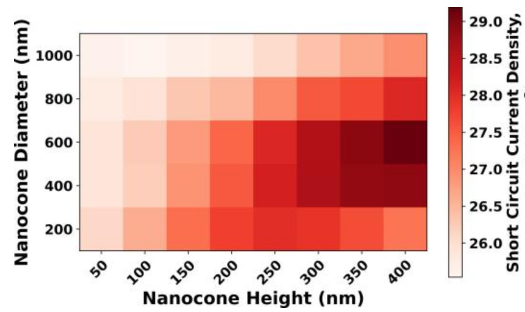

Fig. 5: Colormap representation of short circuit current density (J_{sc}) for nanocone sizes ranging 50-400 nm in height and 200-1000 nm in diameter [J_{sc} of bare CdTe TFSC is 25.95 mA/cm^2].

were done in CHARGE to obtain open circuit voltages (V_{oc}) as discussed in previous studies. The V_{oc} values were then again used for obtaining normalized open circuit voltages ($V_{oc}(n)$). Subsequently, fill factor, which is a parameter that implies the maximum attainable power output from a solar cell, was calculated using methods in previous studies [17] [18]. The fill factor and normalized open circuit voltage were used together to calculate the efficiency (η) and output power (P_{max}) per unit area using equations from previous studies [17] [18]. Lastly, the optical near-field distribution data were obtained and visualized for CdTe TFSCs with nanocone surface texture as discussed in previous studies [17] [18].

III. Results and Discussions

A. Nanocone Diameter and Height Variation Analysis

For the diameter and height variation study of the nanocone texture, the side-to-side pitch of the nanocone as depicted in Fig. 3 was kept constant at 100 nm. Later on upon obtaining the optimal diameter and height, pitch variation of the nanocone was done.

1) Optical Absorption Factor Analysis (g): Nanocone texture of diameters ranging from 200 nm to 1000 nm and heights ranging from 50 nm to 400 nm were considered for comparison with respect to the bare CdTe substrate to calculate the optical absorption factor (g). The sum of the optical absorption factor across 150 wavelength points (λ) within the wavelength range of λ_{min} (400 nm) and λ_{max} (1100 nm) for bare CdTe TFSC was 150 (arbitrary units). From Fig. 4 it is evident that most of the nanocone textured CdS gives a significant enhancement compared to the bare CdTe TFSC case. The best configuration for the highest absorption is seen to be the structure with 600 nm in diameter and 400 nm height which shows about 22.99% (g = 184.49) enhancement compared to the bare CdTe TFSC case (g = 150).

2) Short Circuit Current Analysis (J_{sc}): The short circuit current density (J_{sc}) values for the same set of configurations tend to follow the same pattern as the optical absorption factor (g) values. In Fig. 5, among the different-sized nanocone textures, the nanocone design of 600 nm diameter and 400 nm height gave the highest J_{sc} which is approximately 12.48% (J_{sc} = 29.19 mA/cm^2) enhancement over the bare CdTe TFSC case (J_{sc} = 25.95 mA/cm^2).

3) Open Circuit Voltage Analysis (V_{oc}): Despite the fact that textured surfaces appear to exhibit a certain level of enhancement, the change in V_{oc} is not significant, as shown in Fig. 6 color map. Compared to the bare CdTe TFSC case (V_{oc} = 1.0872 V), the nanocone structures of the same configuration of highest J_{sc} showed an incremental enhancement in V_{oc} (i.e., V_{oc} = 1.0894 V showing a 0.20% enhancement over the bare CdTe TFSC case).

4) Fill Factor Analysis (FF): The fill factor (FF) is one of the significant performance parameters that determine the attributes of a solar cell. In Fig. 7, the FF value trends differently from the previously mentioned highest J_{sc} and V_{oc} structures. In fact, most of the structures of 1000 nm diameter with 200 nm - 350 nm height show almost identical enhancements, having a fill factor around 0.7640 while bare CdTe TFSC have a FF of 0.7625.

5) Output Power Analysis (P_{max}): Output power (P_{max}) refers to the maximum discharge power at optimal operating conditions. In Fig. 8, the optimal design set of diameter 600 nm and a height of 400 nm that previously displayed the optimal J_{sc} and V_{oc} from all the configurations studied, provides the maximum P_{max} of 24.24 mW/cm^2. With respect to

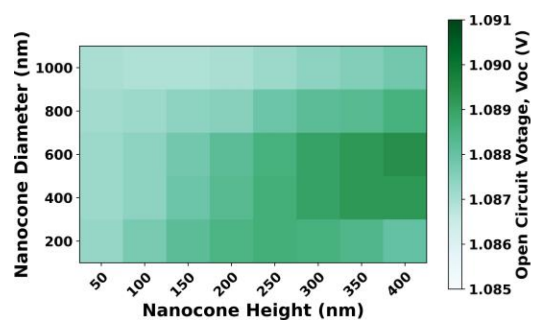

Fig. 6: Colormap of open circuit voltage (V_{oc}) for the nanocone texture ranging from 50-400 nm in height and 200-1000 nm in diameter [V_{oc} of bare CdTe TFSC is 1.087 V].

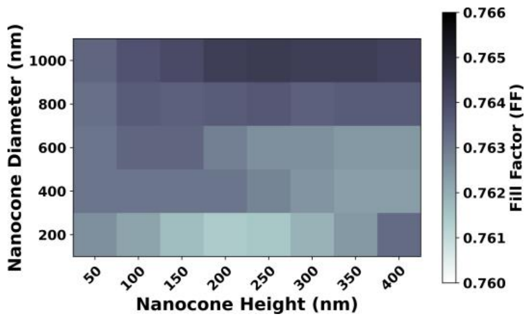

Fig. 7: Colormap interpretation of fill factor (FF) for nanocone texture varied between 50 to 400 nm in height and 200 to 1000 nm in diameter [FF of bare CdTe TFSC is 0.7625].

the bare CdTe TFSC case (i.e., with no surface corrugations), it is a significant enhancement of 12.7% whereas the maximum output power for bare CdTe TFSC is 21.51 mW/cm^2.

6) Efficiency Analysis: Fig. 9 shows the overall efficiency of CdTe TFSC with different-sized nanocone textures on the CdS window layer. Except for the FF, all the other parameters such as J_{sc}, V_{oc} yielded optimal results for the configuration where the nanocone diameter was 600 nm and height was 400 nm. So, it is expected from Fig. 9 that the efficiency of the same structure will be the highest (η = 24.24%) among all the varied sizes of nanocone texture hence significantly elevated from bare substrate (η = 21.51%).

B. Pitch Variation Analysis

The nanocone structure under investigation showed enhanced performance for the diameter of 600 nm and height 400 nm, respectively. The third parameter for this computational study is the pitch which represents edge to edge distance between neighboring nanocone structures in an array. The pitch was varied from 25 nm to 150 nm to find the optimum pitch. From Table I, it can be stated that 75 nm pitch distance was the optimal pitch distance as it yielded greater electrical performance parameter values, such as short circuit current density of 29.56 mA/cm^2 compared to 25.95 mA/cm^2 for bare

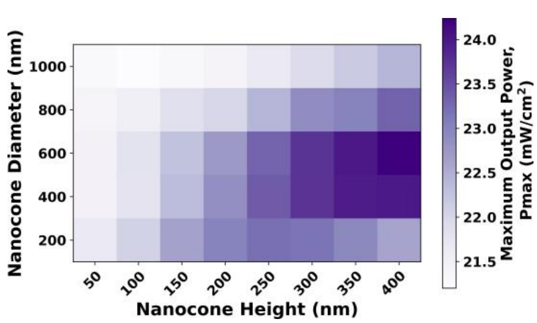

Fig. 8: Colormap interpretation of maximum output power (P_{max}) for nanocone texture ranging from 50-100 nm in height to 200-1000 nm in diameter [P_{max} of bare CdTe TFSC is 21.51 mW/cm^2].

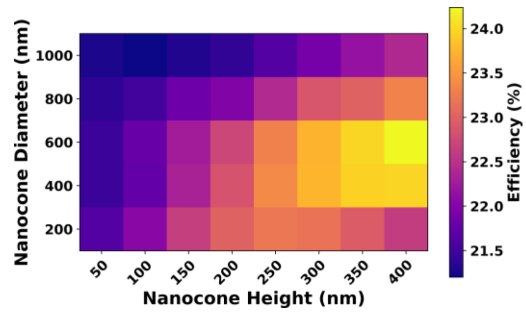

Fig. 9: Efficiency (η) shown in colormap for Nanocones ranging in size from 50-400 nm in height and 200-1000 nm in diameter [η of bare CdTe TFSC is 21.51%].

CdTe TFSC. Similarly efficiency showed a change of 14.13% where it rose from 21.51% for bare CdTe TFSC to 24.55% for CdTe TFSC with nanocone structure.

C. Optical Near-field Analysis

Plotting the optical near-fields gives a visual representation of light matter interaction and how the electromagnetic field is distributed within/around the window and absorbing layer of the CdTe TFSC. In this study, significant enhancements in the optical near-fields were observed for CdTe TFSCs with textured CdS surface as compared to bare CdTe at the incident wavelength of λ = 900 nm as shown in Fig. 10. To generate this optical near-field enhancement image, a two-dimensional monitor was placed along the x-z plane that sliced through the middle of the CdTe TFSC (both with and without the nanocone surface texturing). From Fig. 10, it can be observed that in the region right below the textured CdS nanocone, the light intensity is higher. This suggests significant light trapping within the CdTe absorbing layer, which eventually leads to more electron-hole pair generation resulting in larger photo-current generation. The intensity of the light inside and around the nanocone textured CdTe TFSC has been

TABLE I: Pitch variation study of nanocone texture for the diameter, D = 600 nm and height, H = 400 nm.

Nano-cone Pitch (nm)	**g**	**J_{sc} (mA/cm^2)**	**V_{oc} (V)**	**FF**	**P_{max} (mW/cm^2)**	**η (%)**
Bare CdTe	150	25.95	1.0872	0.7625	21.51	21.51
25	175.28	29.26	1.0894	0.7630	24.32	24.32
50	182.72	29.39	1.0895	0.7626	24.42	24.42
75	188.95	29.56	1.0896	0.7621	24.55	24.55
100	183.77	29.19	1.0894	0.7624	24.24	24.24
125	182.72	29.24	1.0894	0.7626	24.29	24.29
150	175.02	28.98	1.0892	0.7627	24.08	24.08

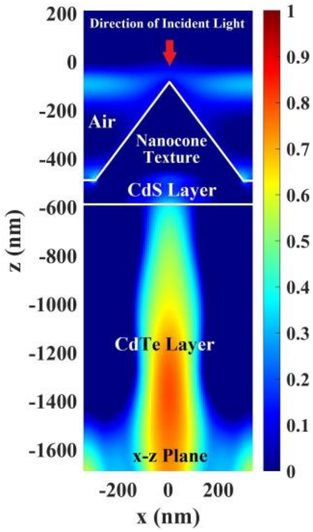

Fig. 10: Optical near-field enhancement image of absorbing substrate with nanocone textured CdS surface at λ = 900 nm.

represented in logarithmic scale where value '1' represents 10-fold enhancement.

D. Comparison with Plasmonic Nanoparticles

1) Absorption Spectra Analysis: In Fig. 11, absorption of bare CdTe TFSCs, CdTe TFSCs with silver (Ag) nanoparticle on the top surface, and CdTe TFSCs configured with textured CdS have been illustrated with an average absorption of 64%, 73% and 82% respectively. The absorption spectra spanned a wavelength region from 400 nm to 1100 nm (which comprises of visible and near-IR region). Previous studies have shown that Ag nanoparticles of 200 nm diameter when placed over top surface of CdTe TFSC exhibit enhanced absorption [7] [19]. These studies have shown that Ag nanoparticles help to significantly enhance light absorption into the CdTe absorbing layer when compared to a bare CdTe TFSC in the visible range of the electromagnetic (EM) spectrum. However, both of

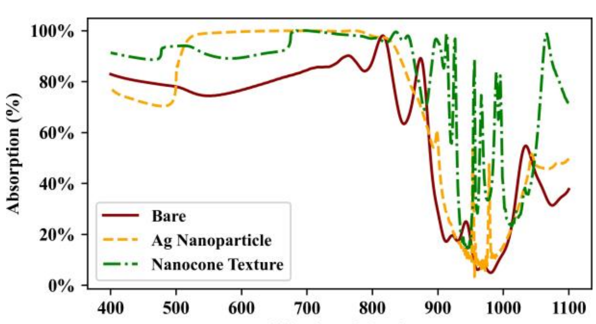

Fig. 11: Absorption spectra over an incident radiation range from 400 nm to 1100 nm for bare CdTe TFSC, CdTe TFSC modified with silver nanoparticle on the top surface and CdTe TFSC with nanocone textured CdS window layer.

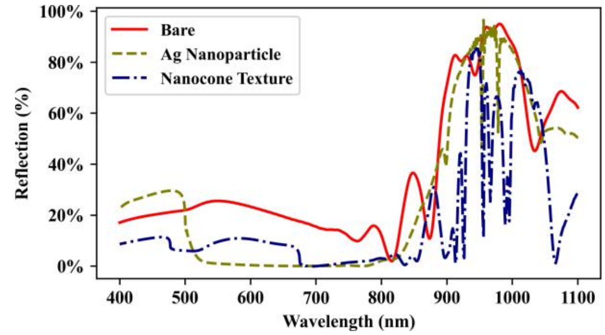

Fig. 12: Reflection spectra over an incident radiation range from 400 nm to 1100 nm for bare CdTe TFSC, CdTe TFSC modified with Ag nanoparticle on top, CdTe TFSC with nanocone textured CdS top surface.

their performance drops in the near-infrared (NIR) region (i.e., $\lambda > 800$ nm). On the contrary, CdTe TFSCs with nanocone-shaped textured CdS showed high absorption over a broad range of the EM spectrum (including the NIR region). This indicates that introducing such type of surface corrugations on the CdS window layer can significantly increase the light absorption capability of CdTe TFSCs in both the the visible and NIR regions. Table II shows the opto-electronic performance parameters of the three types of CdTe TFSCs studied above. It is easily comprehensible from Table II that nanocone textured CdTe TFSCs can be considered as an efficient light trapping structure and a viable solution for enhancing the opto-electronic performance of CdTe TFSCs while also overcoming the hurdle of complex fabrication process that is needed for the coupling of the CdTe TFSCs to plasmonic metal nanoparticles (e.g., Ag, Au, Al, etc.).

2) Reflection spectra analysis: One significant way to improve TFSC performance is to reduce reflection of incident radiation from the top surface (window layer) as the absorbing layer is only few nanometers to few micrometers thick. To

TABLE II: Performance Comparison of Bare CdTe TFSCs, CdTe TFSCs modified with spherical Ag nanoparticles, and nanocone-textured CdTe TFSCs, respectively.

Configuration	**g**	**J_{sc} (mA/cm^2)**	**V_{oc} (V)**	**FF**	**P_{max} (mW/cm^2)**	**η (%)**
Bare CdTe	150	25.95	1.0872	0.7625	21.51	21.51
Ag Spherical Nanoparticle (D=200nm)	164.32	29.01	1.0893	0.7621	24.08	24.08
Nanocone CdS Texture (P=75nm, D=600nm, H=400nm)	188.95	29.56	1.0896	0.7621	24.55	24.55

have better understanding of this phenomenon, the reflection spectra has been generated in order to compare the reflection of bare CdTe TFSCs, CdTe TFSCs with Ag nanoparticles on top and CdTe TFSC with nanocone-textured CdS surface over a broad wavelength range from 400 nm to 1100 nm. From Fig. 12, it can be observed that in the visible region from $\lambda = 500$ nm to $\lambda = 800$ nm, nanocone textured CdS is a more desirable candidate to reduce top surface reflection as it has brought down reflection to only 18% compared to both bare and nanoparticle-coupled CdTe TFSCs, which hold 36% and 27% of overall average reflection respectively.

IV. Conclusion

This computational study focuses on reducing the surface reflective loss in Cadmium Telluride thin-film solar cells (CdTe TFSCs) by introducing arrays of nanocone-shaped surface textures on the CdS window layer. Optimization of nanocone morphology was done by varying the nanocone diameter from 200 nm to 1000 nm, height from 50 nm to 400 nm, and the side-to-side distance between neighboring nanocones (pitch) from 25 nm to 150 nm. The increase in short-circuit current density (J_{sc}) compared to the bare CdTe substrate (i.e., flat top surface with no texturing) has been observed in most of the configuration of surface texturing investigated. The highest (J_{sc}) achieved was for the nanocone design having a diameter, height and pitch of 600 nm, 400 nm and 75 nm respectively which showed a 13.91% enhancement over the bare CdTe TFSC case. Approximately 14.13% enhancement in efficiency was obtained for the same nanocone texture configuration as well. An additional comparison with CdTe TFSCs incorporated with optimal plasmonic metal nanoparticles (silver) was also performed because to date, plasmonic nanoparticles have been commonly used to enhance the opto-electronic performance of solar cells. It has been found that the CdTe TFSCs modified with nanocone-shaped surface textures showed superior opto-electronic performance compared to CdTe TFSCs coupled to plasmonic nanoparticles. This study shows that certain types of surface texturing on top surface of the CdTe TFSCs can be a more attractive option than incorporating plasmonic metal nanostructures (thus also avoiding unnecessary fabrication complexities) to get optimal performances from TFSCs. Additionally, an analysis of absorption and reflection spectra for bare CdTe TFSCs and CdTe TFSCs modified with surface texturing and plasmonic metal nanoparticles, respectively, was also presented. This study shows the immense potential of using surface texturing at the nanoscale on the top surface of solar cells as an attractive option to increase incident light absorption (by reducing the reflection from the top surface) within the absorbing substrate (i.e., CdTe layer) over a broad wavelength range and thus generating increased output current. Thus, CdTe TFSCs hold immense potential to be a sustainable technology and contribute to efficient renewable energy production. Future studies would be focused on optimizing multiple morphological parameters of the texturing structures at the same time.

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