Use of Nano-grating Structures Embedded within the Absorbing Substrate to Optimize the Efficiency of Cadmium Telluride Thin-film Solar Cells

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***Abstract*—Thin film solar cells (TFSCs) are one of the leading candidates to reduce the cost of photovoltaic production. However, low absorption coefficient due to relatively low light absorber layer thickness can limit the performance of TFSCs. To address these problems, this study computationally investigates the opto-electronic performance of Cadmium Telluride (CdTe) TFSCs with a metallic nano-grating structure embedded within the absorber layer. The finite-difference time-domain (FDTD) numerical analysis technique was used to computationally analyze different solar cell performance parameters with and without the nano-grating structure. Furthermore, an artificial intelligence (AI) technique, namely particle swarm optimization algorithm (PSO) was used to determine the optimum nano-grating configuration with respect to nano-grating height, angle and duty cycle. The results suggest that the short circuit current density increased by 20.72% while the solar cell efficiency yielded an increase of 21.66% for the Cadmium Telluride (CdTe) thin film solar cells (TFSCs) with the optimized nano-grating structure in comparison to a bare CdTe TFSC with no nano-grating. The results indicate that an important role can be played by such nano-grating structures to significantly enhance the opto-electronic performance of TFSCs and this process can be optimized by the use of AI techniques.**

***Keywords*—Cadmium Telluride, thin-film solar cell, nano-grating, finite-difference time-domain, FDTD, particle swarm optimization, artificial intelligence, plasmonics, renewable energy.**

I. INTRODUCTION

To meet the global energy requirement, currently a lot of research is targeted at developing photovoltaic systems using solar cells with high optical, electrical and thermal properties [1]. Among them, crystalline silicon solar cell tops the list to achieve high efficiency [2]. However, the need for thin film solar cells (TFSCs) has significantly increased which is required in different mobile electronic devices and other nanoscale applications (e.g., cell phones, tablets, smart-watches, pedometers, monitors for heart rate, quality of sleep and stairs climbed, etc.) which has reduced the dependence on Si-based solar cells as it requires thick absorber layers (due to the relatively moderate light absorption capacity of Si) [3]. It is now well established that Cadmium Telluride (CdTe) is preferred over amorphous Si for the absorber layer of TFSCs, because CdTe has an ideal band gap (1.45eV), and an increased absorption coefficient of 10^6 cm^{-1} in 300K (room temperature) in the visible to near-infrared wavelength range [4]. In TFSCs, the absorber layer thickness ranges from a few nanometers to a few microns [5]. Hence, when designing TFSCs, one of the main challenges is to improve the light trapping inside the absorber layer over a wide range of wavelengths for the incident solar radiation. TFSCs with efficient light trapping offers a number of advantages. Firstly, the material requirement is reduced. Secondly, the reduction in absorber layer thickness improves the collection efficiency of electron-hole pairs [6], [7]. Finally, thin film solar cells has the added advantage of increasing the packing density of solar cells for mass scale production [8]. Effective light trapping in TFSCs falls under two categories, the first being reduction of light reflection in the front surface and the second involves increasing the optical path length of the absorbed light within the absorber layer of TFSCs (which allows for increased opportunity of absorption of the light and thus increased chances of electron-hole pair generation). Recently, nanostructures such as plasmonic metal nanoparticles [9], [10], ordered nano-rods and nano-pillars [11], metallic nano-gratings [12], are being investigated in various ways to increase light absorption within the absorber layer of solar cells. Thus, by incorporating these nanostructures, TFSCs can be designed which are thick enough for efficient photon absorption and thin enough for electron motion simultaneously, which will enhance overall efficiency of TFSCs. In this computational study, the opto-electronic performance enhancement of CdTe TFSCs is enhanced by embedding a metallic nano-grating structure inside the absorber layer of CdTe TFSCs which demonstrated increased broad-band light absorption in comparison to bare CdTe TFSCs which had no nano-grating structure embedded. This study involves two parts where initially the material of the nano-grating material was decided based on optical and electrical simulation results using the finite-difference time-domain (FDTD) method. Secondly, particle swarm optimization algorithm was used for determining the optimum nano-grating configuration [13]. It is shown that CdTe TFSCs incorporating metallic nano-gratings designed by the methods mentioned above show increased short circuit current density and efficiency when compared to bare CdTe TFSCs (i.e., with

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no nano-grating).

II. Material and Methods

A. Simulation Setup

FDTD Solutions and CHARGE from Ansys Lumerical were used for used for all simulations in this study [14]. FDTD Solutions was used to do optical simulations based on which optical generation file was generated. This file was later used during CHARGE simulation for extracting electrical performance parameter values.

Fig. 1 shows a three-dimensional (3D) schematic of the setup of the FDTD simulation region where light-solar cell interactions were investigated. Here, the proposed CdTe TFSCs has a 100nm CdS window layer followed by 1500nm CdTe absorber layer. For this study, built in metallic nano-grating structure(s) present in the FDTD Simulations have been embedded into the absorber layer which had a total period of 600nm and height of 120nm. Different parameters such as nano-grating material, nano-grating height, duty cycle and angle were varied using the built in nano-grating structure. For incident radiation, a plane wave of AM 1.5G solar spectrum with light intensity 1000 W/m^2 was taken [15]. The wavelength of incident radiation was set between 400nm to 1100nm to study the broadband absorption outside the visible spectrum.

Fig. 2 shows a three-dimensional (3D) schematic of the CHARGE simulation region of CdTe TFSCs used to generate values of the electrical performance parameters of the CdTe TFSCs. Previous studies suggest doping concentration to be 1.0×10^{15} cm^{-3} for CdS layer and 1.5×10^{17} cm^{-3} for CdTe layer which was the n-type and p-type layer in this study [16]. Voltage sweeping was done within a range of 0 to 1.2 V having two silver (Ag) contacts as metallic contacts.

B. Numerical Background

All simulations were carried out for a wavelength range of 400nm to 1100nm since this is the commonly used wavelength range for most of the solar cell simulations. Short circuit density (J_{sc}), which is reliant on the wavelength of the incident radiation and the power absorbed by a solar cell was calculated using the equation mentioned previously [16]. CHARGE was used to conduct electrical simulations, which generated the open circuit voltage (V_{oc}) values. The V_{oc} values were further used to calculate the normalized open circuit voltage ($V_{oc}(n)$). Additionally, the fill factor (FF), a parameter indicative of the maximum obtainable power output from a solar cell, was calculated using the equation used previously [17]. Subsequently, normalized open circuit voltage ($V_{oc}(n)$) and fill factor (FF) were used to compute the output power (P_{out}) per unit area and efficiency (η) using their corresponding equations shown previously [17]. Lastly, for computations regarding the optical near-fields, field distribution data were obtained for both bare CdTe TFSCs and CdTe TFSCs coupled with embedded optimal nano-grating structure. Dividing the nano-grating incorporated near-field by bare substrate near-field gave the enhanced near-field plot. This allowed the calculation of enhanced electric field distributions near the vicinity of nano-grating and substrate at a greater detail.

III. Results and Discussions

A. Nano-grating Material Study

1) Short Circuit Current Analysis: Fig. 3 compares the short circuit current density (J_{sc}), the maximum amount of current of solar cell when short circuited, for five nano-grating materials along with the bare CdTe substrate (i.e., with no nano-grating incorporated inside) [17].

Fig. 3 clearly shows that all nano-grating material returns higher value of J_{sc} compared to the bare CdTe substrate. Furthermore, metallic nano-gratings exhibit better electron-hole pair generation compared to an insulating dielectric nano-grating SiO_2. Metals like Ag, Au, Al, and Ti, when used as the nano-grating material, give J_{sc} values of 29.36, 29.43, 29.74, and 31.34 mA/cm^2 respectively whereas metal oxides such as SiO_2 provide J_{sc} of 26.75 mA/cm^2. Hence, Ti gives the highest J_{sc} value.

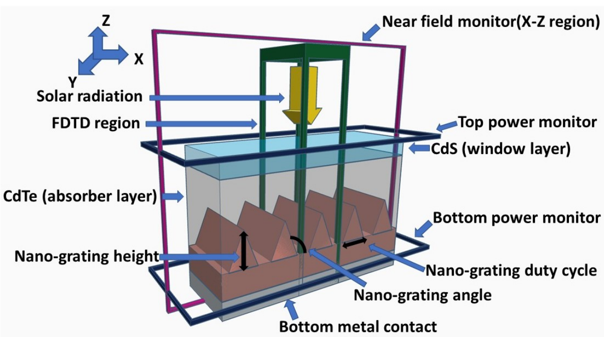

Fig. 1. 3D schematic of FDTD simulation setup of nano-grating structure embedded into the absorber layer of CdTe TFSCs to study optical parameters.

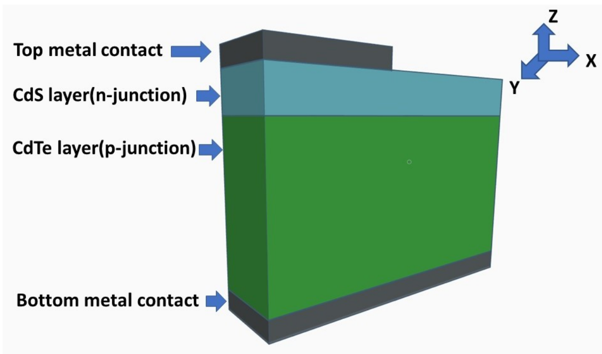

Fig. 2. 3D schematic of CHARGE simulation setup of CdTe TFSCs to study electrical performance parameters.

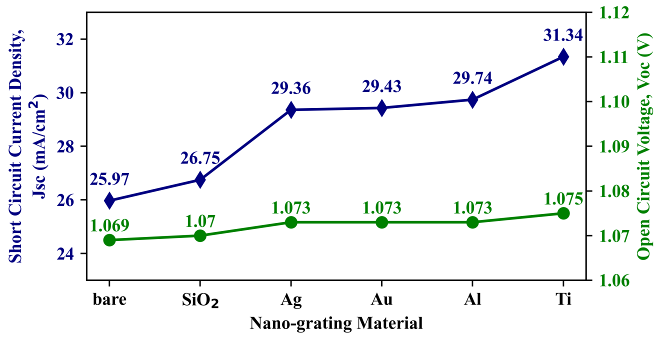

Fig. 3. Short-Circuit Current Density (J_{sc}) and Open Circuit Voltage (V_{oc}) value for CdTe TFSCs when incorporated with nano-grating of different materials: (a) bare, (b) SiO_2, (c) Ag, (d) Au, (e) Al, and (f) Ti.

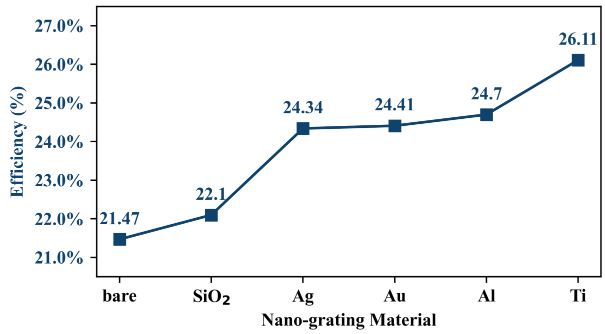

Fig. 5. Percentage Efficiency (η) of CdTe TFSCs embedded with different nano-grating materials: (a) bare, (b) SiO_2, (c) Ag, (d) Au, (e) Al, and (f) Ti.

2) Open Circuit Voltage Analysis: Unlike J_{sc}, the change in V_{oc} is not significant as seen in Fig. 3. Ti nano-grating material yields the highest V_{oc} which is 1.075 V. The remaining nano-grating materials also provide comparable V_{oc} to Ti (i.e., 1.073 V for Ag, Al, and Au nano-grating material each, and 1.070 V for SiO_2) while the bare CdTe TFSCs has a V_{oc} of 1.069 V.

3) Fill Factor Analysis: Being one of the significant performance parameters, the fill factor (FF) determines the quality of a solar cell. Fig. 4 compares the FF and P_{out} values for five nano-grating materials along with the bare CdTe substrate. The variation of FF values over different nano-grating materials shows no significant change like V_{oc} as expected. The highest fill factor was yielded by Ti nano-grating material, 0.775, while SiO_2 has the lowest fill factor of 0.772 (actually less than the bare CdTe TFSC by a very little margin).

4) Output Power Analysis: The maximum amount of power per unit area that a solar cell produces can be put under the name of output power, (P_{out}). In fact, it is the maximum output power in the optimal operating condition [17].

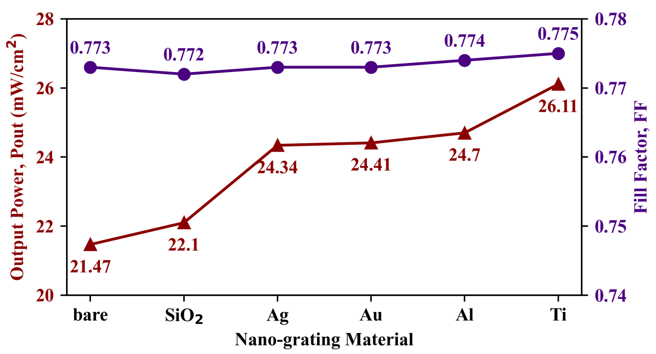

Fig. 4. Fill Factor (FF) and Output Power (P_{out}) value for CdTe TFSCs when incorporated with nano-grating of different materials: (a) bare, (b) SiO_2, (c) Ag, (d) Au, (e) Al, and (f) Ti.

As shown in Fig. 4, CdTe TFSCs incorporated with Ti nano-grating gives the maximum output power of 26.11 mW/cm^2 compared to other nano-grating materials. On the other hand, Ag, Au, and Al nano-grating material provides comparable output power, 24.34, 24.41, and 24.70 mW/cm^2 respectively. The least-performing nano-grating material among all is SiO_2, delivering 22.10 mW/cm^2.

5) Efficiency Analysis: The efficiency (η) of a solar cell indicates how effectively a solar cell can convert solar energy into electrical energy. It is the ratio of the maximum output electrical power at the solar irradiance of AM 1.5G [17].

Fig. 5 shows the overall efficiency of CdTe TFSC embedded with different nano-grating materials and compares the results with the bare CdTe TFSC. It can clearly be seen from Fig. 4 and Fig. 5 that the efficiency curve follows the same pattern as the maximum output power, P_{out}. Similar to the maximum output power curve, Ti nano-grating delivers the highest efficiency of 26.11%, which is 21.62% higher than that of the bare CdTe substrate.

B. Optimizing Nano-grating Configuration Using Particle Swarm Optimization (PSO)

The parameters which were investigated for this computational study were nano-grating height, angle and duty cycle. While the first two parameters are self-explanatory from Fig. 6, the latter (i.e., duty cycle) is demonstrated using Fig. 7 where four different duty cycles of the nano-grating structure were illustrated. Here duty cycle represents part of nano-grating structure along the x-span for which it will have the grating present. Although Ti material has been found to be a promising nano-grating material based on the configuration set by literature review, the optimum configuration of the nano-grating structure can further enhance the results [18]. Hence, particle swarm optimization (PSO) algorithm was used, which is a built-in feature of FDTD Solutions.

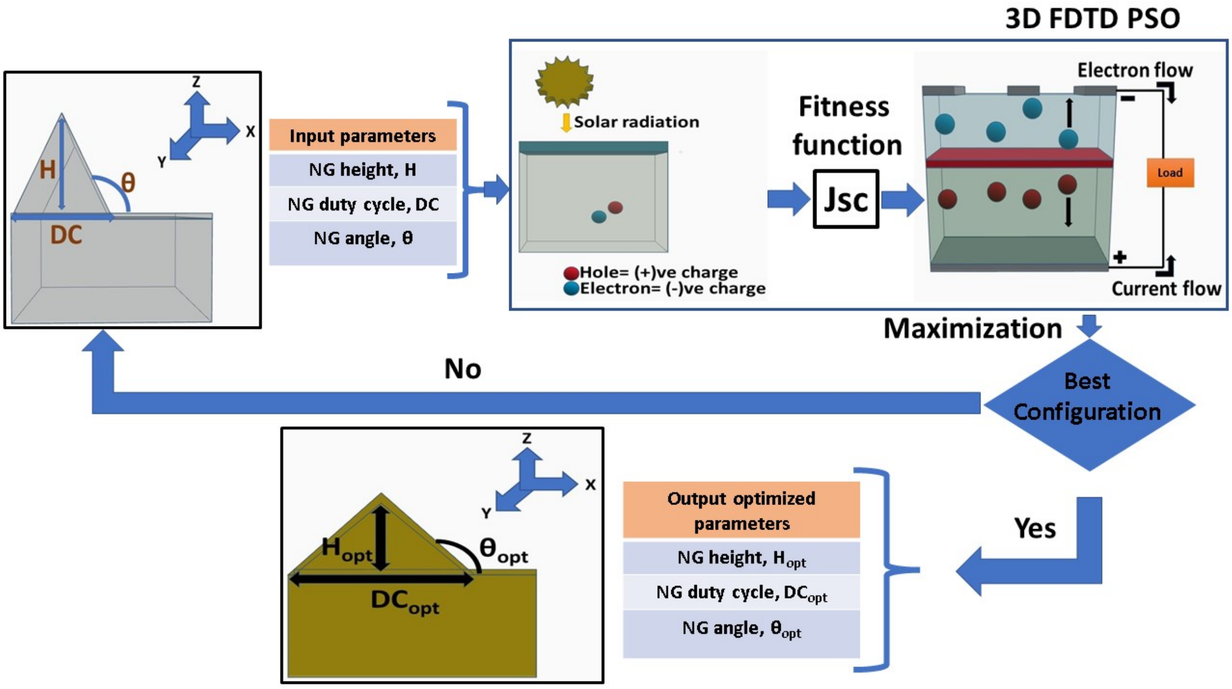

Fig. 6. Operational behavior of the Particle Swarm Optimization (PSO) algorithm used to find out the optimal nano-grating structure of CdTe TFSCs.

The PSO algorithm is fast and with few adjustable parameters, it can optimize any non-linear functions. This optimization technique which is inspired by social behavior of birds flocking together suggests change of set parameters in a randomized mannner to achieve the maximum or minimum of a well-defined fitness function [19]. Here each particle position represents a multi-dimensional vector which in this case are the nano-grating parameters whose optimum value was found by using the PSO algorithm. The fitness function was set to be short circuit current density (J_{sc}). Here, each particle position was updated from one simulation to another by two factors which are mainly best position of each particle and best position for all particles, more commonly called local best (L_i) and global best (G_i) respectively. The iterations were run based on following equations [13]:

$$V_{i+1} = V_i + C_1 r_1 (L_i - P_i) + C_2 r_2 (G_i - P_i) \tag{1}$$

$$P_{i+1} = P_i + V_{i+1} \tag{2}$$

where r_1, r_2 represent any random numbers between [0,1] and C_1, C_2 represent cognitive and social behavior factor respectively. V_i represents particle velocity depending on particle position, P_i. The nano-grating height, angle and duty cycle were described within the vector, P_i (such that P_i=nano-grating height, angle and duty cycle). The optimization range of the said nano-grating parameters were kept between 0.1 - 0.9 for duty cycle, 10° - 90° for angle and 80nm - 130nm for nano-grating height based on literature review [18]. Due to computational limitations, the generation number was set to 10 where 15 simulations ran within each generation. Yet,

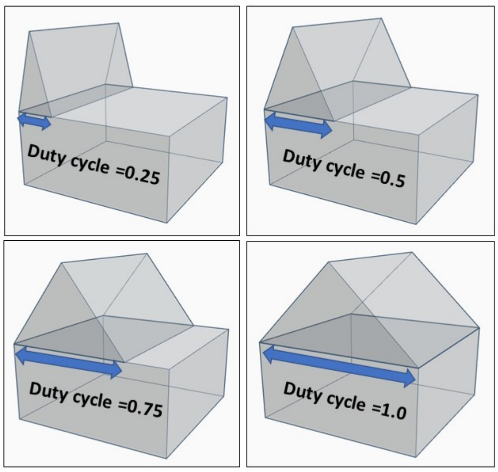

Fig. 7. Varying duty cycle (0.25, 0.5, 0.75, 1.0) of the nano-grating structure

TABLE I
OPTIMIZED PARAMETER OF NANO-GRATING

Nano-grating Parameter	Parameter Range	Optimized Parameter Value
Height	80 - 130nm	130nm
Angle	10° - 90°	34.99°
Duty Cycle	0.1 - 0.9	0.67

TABLE II
COMPARISON BETWEEN BARE AND OPTIMIZED CdTe TFSCs

Configuration	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	P_{out} (mW/cm^2)	Efficiency, η
Bare CdTe	25.97	1.069	0.773	21.47	21.47%
CdTe with optimal nano-grating structure	31.35	1.075	0.775	26.12	26.12%

it was observed that the fitness function which is J_{sc} in this case reached maximum possible value within said number of generations. Fig. 6 illustrates how the PSO algorithm works for finding the optimized value and Table I represents the optimized configuration value for investigated nano-grating parameters. Table II compares the performance parameters of the CdTe TFSCs with and without the optimized nano-grating structure. Performance enhancement was found to be 21.66% for solar cell efficiency (η) whereas the enhancement value was 20.72% for short circuit current density (J_{sc}).

1) Absorbance Spectra Analysis: Fig. 8 illustrates the absorbance spectra of bare CdTe TFSCs and CdTe TFSCs embedded with optimized nano-grating structure. It can be observed that the bare CdTe TFSCs exhibit poor absorption in the near-infrared region, whereas the optimized CdTe TFSCs exhibit significant enhancement in the near-infrared region (i.e., between 900nm-1100nm). The design proposed in this study shows significant absorption when compared to its bare CdTe TFSC counterpart. This suggests that the proposed TFSCs can show enhanced performance for a wider solar spectrum, thus increasing the possibility of harnessing more solar power as compared to bare CdTe TFSCs.

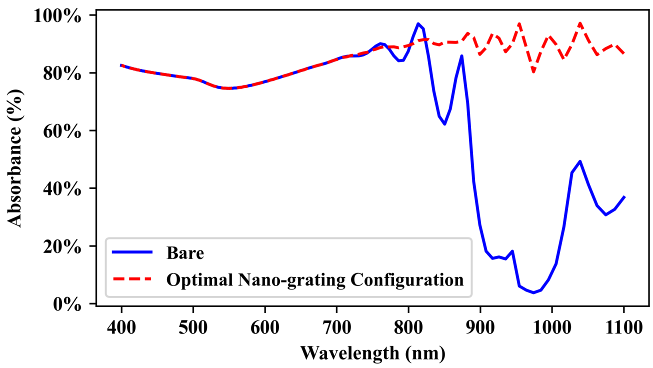

Fig. 8. Absorption spectra for bare CdTe TFSC and CdTe TFSC embedded with the optimal nano-grating configuration between the wavelength of λ_1 = 400 nm to λ_2 = 1100 nm.

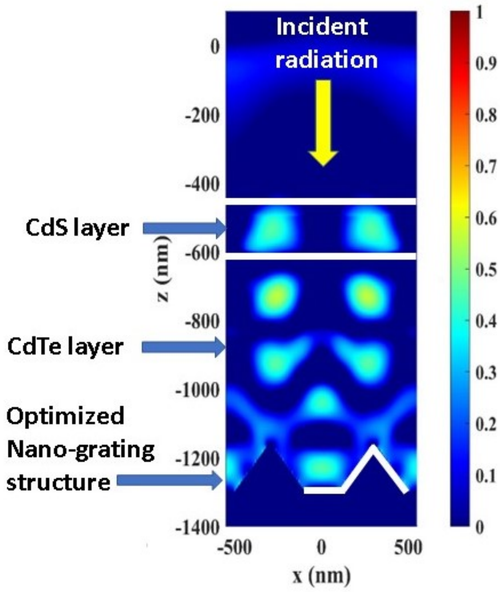

Fig. 9. Enhancements of optical near-field (at λ = 970 nm) throughout the substrate for optimal nano-grating configuration in CdTe TFSCs.

2) Optical Near-Field Analysis: The optical near-field of a solar cell provides a visual interpretation of electromagnetic field intensity distributions in important regions of the CdTe absorbing substrate.

Fig. 9 shows the optical near-field enhancement for CdTe TFSCs embedded with the PSO algorithm generated optimal nano-grating structure of Ti nano-grating material. During the simulation, a two-dimensional near-field monitor was placed to record incident light intensity data along the x-z plane as demonstrated in fig. 1. The optical near-field enhancement image was computed in a manner that has been extensively reported previously [4], [9], [10].

A single wavelength of 970 nm was chosen to generate the optical near-field for this nano-grating configuration due to the fact that the highest absorption enhancement was achieved about this wavelength compared to the bare substrate as seen in Fig. 8. The light intensity for enhancement has been chosen in a 10-base logarithmic scale, where a dark red electromagnetic field valuing 1 would mean at least a 10-fold enhancement. From Fig. 9 it can be seen, being a plasmonic material, Ti nano-grating are providing enhancement of light within its immediate vicinity around the bottom of the CdTe absorbing substrate. Furthermore, multiple nano-grating units are contributing to constructive interference of light covering more areas of the upper light-absorbing substrate. These two effects combined enhance the electromagnetic field significantly and increase the optical path length as well, resulting in increased electron-hole pairs (i.e., current) generations.

IV. Conclusion

This computational study investigates the potential for incorporating metallic nano-grating structure within the absorber layer of CdTe TFSCs for enhanced light trapping and absorption. Initially, finite-difference time-domain (FDTD) simulations were carried out for material selection of nano-grating structure where materials investigated were SiO_2, Ag, Au, Al and Ti. Ti was shown to be the best candidate for nano-grating material (among the materials investigated) where the performance enhancement compared to a bare CdTe TFSC (i.e., with no embedded nano-grating) was found to be 20.68% for short circuit current density (J_{sc}) and 21.62% for solar cell efficiency (η). Subsequently, based on these results, the, Ti nano-grating structure was further optimized using particle swarm optimization algorithm (PSO) for designing the optimal configuration for the nano-grating structure with respect to nano-grating height, angle and duty cycle. The optimized structure further enhanced the opto-electronic performance which yielded percentage change of 20.72% for short circuit current density (J_{sc}) and 21.66% for solar cell efficiency (η), respectively compared to the bare CdTe TFSC. The proposed structure of CdTe TFSCs shows significant absorption enhancement in the longer wavelengths (i.e., near-infrared regions approximately from 900nm-1100nm) where the performance dropped significantly for bare CdTe TFSCs (i.e., without any nano-gratings. Future studies will involve investigating the effects of coating the nano-grating structure with novel nanomaterials like graphene, varying the position of the nano-grating structure inside the absorbing substrate, and placement of plasmonic metal nanoparticles on top of the absorbing substrate to even further enhance the performance of solar cells. Additionally, future studies are also planned where other artificial intelligence (AI) optimization techniques (e.g., Genetic Algorithm, Grey Wolf Optimization (GWO) etc.) will be implemented to design improved nano-gratings and/or other nanostructures to further improve the efficiency of solar cells.

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