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FINITE DIFFERENCE TIME DOMAIN SIMULATION OF LIGHT TRAPPING IN A GaAs COMPLEX STRUCTURE

MOHAMMED M. SHABAT[1], NADARA S. El-SAMAK[1], DANIEL M. SCHAADT[2]

[1] Islamic University of Gaza, Physics Department, Gaza, P.O. Box 108, Gaza Strip, Palestinian Authority
E-mail: shabatm@gmail.com, shabat@iugaza.edu.ps
[2] Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

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Abstract. We theoretically investigate the effects of Gallium Arsenide (GaAs) as an absorbing material in a complex waveguide structure model. Finite Difference Time Domain (FDTD) method is used to discretize the Maxwell's curl equations for the proposed structure. A comparison between Amorphous Silicon (a-Si) and GaAs as absorbing materials is presented through the computation of the absorption spectra. It has been realized that GaAs is still a promising candidate to be used in the waveguide structure models through maximizing the absorption and minimizing the reflectance in the proposed waveguide structure.

Key words: Finite Difference Time Domain method (FDTD), Gallium Arsenide (GaAs), thin film complex structure, surface plasmons.

1. INTRODUCTION

Solar cells provide a renewable and clean energy by converting the sunlight to electricity [1–8]. However, it is important to reduce the cost of the solar cell and increase the efficiency in order to be considered as a reliable energy source. Thin film solar cell technology is facing difficulties due to its low energy conversion efficiency. Over many years, a lot of researchers worked on improving both the efficiency and the cost of solar cells. Much efforts and considerable research have been focused on Amorphous Silicon (a-Si) and Gallium Arsenide (GaAs) material [9–11] in solar energy technology to achieve high efficiency because of their high absorption, anti-radiation ability, and good semiconductor band gap leading to higher photoelectric conversion. A complete design for nanostructured solar cells containing GaAs junction and AlGaAs window has been demonstrated to achieve high absorption [11]. GaAs solar cell structures have been used in models of double anti-reflection coating containing a nanoporous anodic aluminum oxide layer. GaAs materials with ZnO films have been also demonstrated as solar cells models to get a good efficiency [12]. Compared with a-Si, GaAs is widely used as an absorbing material in solar cells. GaAs is characterized by its higher photoelectric conversion efficiency and anti-radiation ability. GaAs thin film solar cell structures with periodic silver nanoparticles (NPs) have been designed to get higher absorption enhancement [13]. The light trapping effects in InGaAs/GaAs quantum well solar cells on wavelength and incident angle have also experimentally been characterized and analyzed.

Solar cells efficiency depends on the concept, technique, and mechanism of Surface Plasmons Resonances (SPRs), where the SPRs are the resultant of the interaction of electromagnetic waves with free electrons of metal. In other terms, SPRs are considered as collective oscillations of the free electrons that are restricted to the surface and interact strongly with light caused by the polarization. SPRs are used and implemented to improve the absorption efficiency of the thin film solar cells. SPRs occur at the interface between a dielectric with a positive dielectric constant $\varepsilon_r{}^d$ and a metal with a negative dielectric constant $\varepsilon_r{}^m$. The relation $\mathrm{Re}(\varepsilon_r{}^m) > \varepsilon_r{}^d$ must be satisfied in order to excite SPRs. Many studies have shown the importance of Plasmonics in generating solar cell energy [14–19]. Schaadt, Feng, and Yu [20] have reported the mechanism of surface plasmons in some waveguide structure containing semiconductors and investigated the optical absorption *via* surface plasmon excitation in metal NPs.

In this work, SPRs have been generated through the considered waveguide structure between the Au electrodes the a-Si medium leading to a solar cell model. The thin active layer of GaAs allows the incident light to be well absorbed, which increases the efficiency of the solar cell. In our model, we are not simulating a whole solar cell but rather work on the concept for better light trapping.

2. MODEL AND THEORY

This work contains a theoretical analysis and computations for a strip waveguide structure which builds up on the concept, notations and in somehow on the approach presented in [21]. To investigate the performance of GaAs in the considered waveguide structure as absorbing material, we consider a complex waveguide model as a two-dimensional plasmonic thin-film silicon structure, as shown in Fig. 1. For the proposed structure, all materials are non-magnetic (*i.e.* $\mu_r = 1$). SPRs are excited by the metallic periodic nanostructures and subwavelength scatters. The unit cell of the plasmonic thin-film solar cell is shown in Fig. 1. Let us consider the complex structure as consisting of the GaAs as the absorbing medium. The structure contains four layers, which include indium tin oxide (ITO), absorbing materials, Au electrodes, and substrate with thicknesses of d_1, d_2, d_3, and d_4, respectively. The distance between the two adjacent strips is d_5 and the periodicity is *P*. The PML and Mur absorbing boundary conditions are imposed at the top and the bottom of the solar cell structure. The periodic boundary conditions (PBC) are employed at the left and right sides of the unit cell. TM-polarized incident light is coming from the air on the proposed waveguide structure with the electromagnetic components of H_z, E_x and E_y. The TM-polarized incident light through the considered cell structure generates some kind of surface plasmons between the two media, the absorbing medium and Au medium. The $\exp(j\omega t)$ time convention is used, where ω is the angular frequency of the light. The substrate is a-Si in both studied cases and throughout the present work.

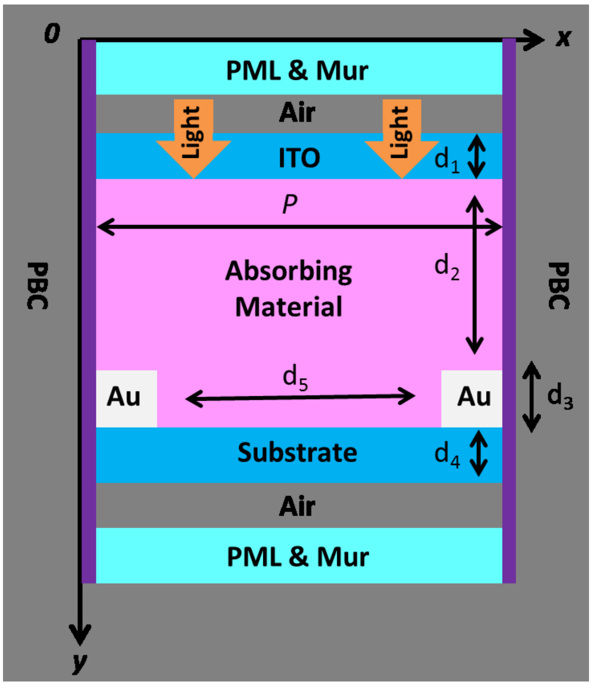

Fig. 1 – Schematic diagram of the unit cell of the plasmonic thin-film solar cell (after Ref. [22]).

3. SIMULATION AND THEORETICAL RESULTS

There are many various methods and approaches for dealing and treating the behavior of light through the complex solar cell waveguide structure as the Transfer Matrix (TM) method [22–24] and the Finite Difference Time Domain (FDTD) method [24–29]. The FDTD method is one of the most effective numerical methods in the study of waveguides [16, 17]. As a direct solution to the Maxwell's Equations, FDTD method offers a simple way to model the complex periodic structures. FDTD method is based on numerical solution of Maxwell's curl equations. In this method, the time and space derivatives are approximated using finite difference approximations. The ***E*** and ***H*** fields are evaluated iteratively at alternative half-time steps. The FDTD algorithm was first proposed by Kane Yee in 1966, and then improved by others in early 70s [24–29]. The algorithm describes the basics of the FDTD model to solve Maxwell's curl equations in time domain. To determine the optimal proposed waveguide structure model for solar cells, a numerical simulation is performed. For the numerical computation, the operating desired wavelength of the light varies between 300 nm and 900 nm in the visible region. We use the following parameters for the film layer refractive index. The average dielectric permittivity for GaAs is taken 3.8 in our computation [23, 30]. The numerical simulation based on the FDTD method is performed to discretize the Maxwell's equations to find out the reflection, transmission, and absorption spectra. The PML and Mur [27] boundary conditions are imposed as usually to absorb all incident light on the structure boundaries. For the two-dimensional thin film solar cell with periodic structure, as shown in Fig. 1, the absorbing medium is GaAs, the electrode is Au, and the substrate is SiO_2. The geometric parameters of the proposed structure are set as $d_1 = 25$ nm, $d_3 = 40$ nm, $d_4 = 30$ nm, $d_5 = 100$ nm, and with a period of P = 200 nm. The y-directed incident field is the TM, p-polarized plane wave with the amplitude of 1 and the frequency spectrum from 400 nm to 800 nm. The spatial step is set to $\Delta_x = \Delta_y$ = 0.5 nm. Figure 2 illustrates the reflectance, transmittance, and absorption spectra *versus* the operation wavelength of the desired effective range of light for the thickness of the absorbing material $d_2 = 160$ nm. It can be noticed that a strong optical absorption is observed from 550 nm to 640 nm and in the same wavelength range, the minimum reflection has been noticed. The other reflection spectra have also been realized at 800 nm. The noticeable feature of changing the thickness of the absorbing material to $d_2 = 120$ nm is shown in Fig. 3. Both figures showed a much lower reflectance with a large energy range including the short-wavelength, visible, and infrared regions of the solar spectrum. The results shown in Figs. 2 and 3 clearly proved the conventional theory of the light propagation through the waveguide structure system as $R(\lambda) + T(\lambda) + A(\lambda) = 1$.

The computed absorption spectra are displayed in Fig. 4 for different values of the thickness of the absorbing materials: $d_2 = 120$ nm, $d_2 = 160$ nm, and $d_2 = 200$ nm. The influence of the thickness of the absorbing materials on the absorption spectra is also investigated and illustrated in Fig. 4; it has been found that when the thickness of the absorbing materials increases, the maximum peak is shifting toward the increasing of the operating wavelength, thus shifting from 550 nm at the thickness of 120 nm of the absorbing material to 830 nm at the thickness of 200 nm of the absorbing medium. Figure 5 displays the absorption spectra of the light through the strip waveguide structure model containing two different absorbing media, a-Si and GaAs, for comparison. This figure shows that the structure containing GaAs as the absorbing medium exhibits higher absorption values than the structure containing a-Si for a large range of the operating wavelengths and has two pronounced peaks of absorption.

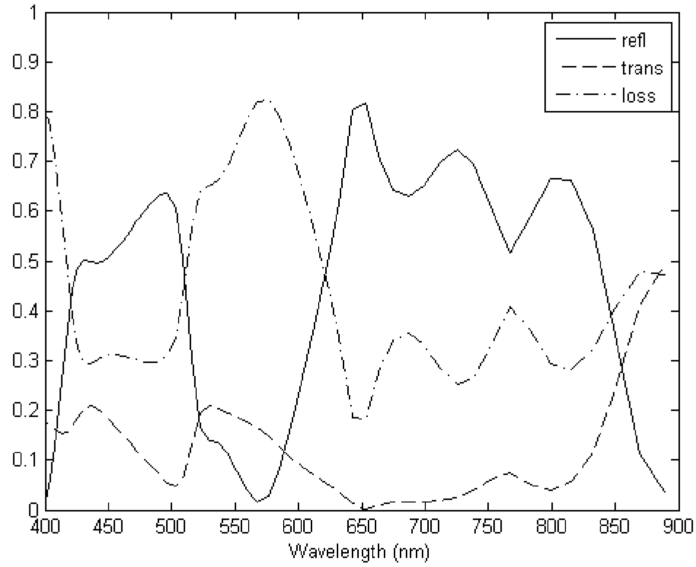

Fig. 2 – Computed reflectance, transmittance, and absorption *versus* the operating wavelength, in the proposed structure containing GaAs as absorbing medium with thickness d_2 = 160 nm.

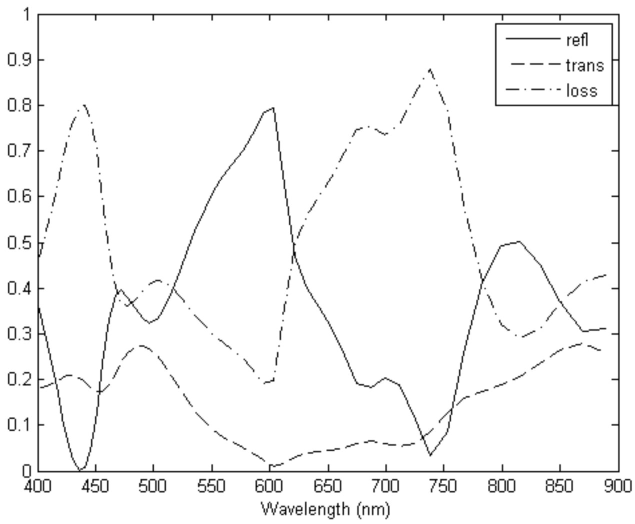

Fig. 3 – Computed reflectance, transmittance, and absorption *versus* the operating wavelength in the proposed structure containing GaAs as absorbing medium with thickness d_2 = 120 nm.

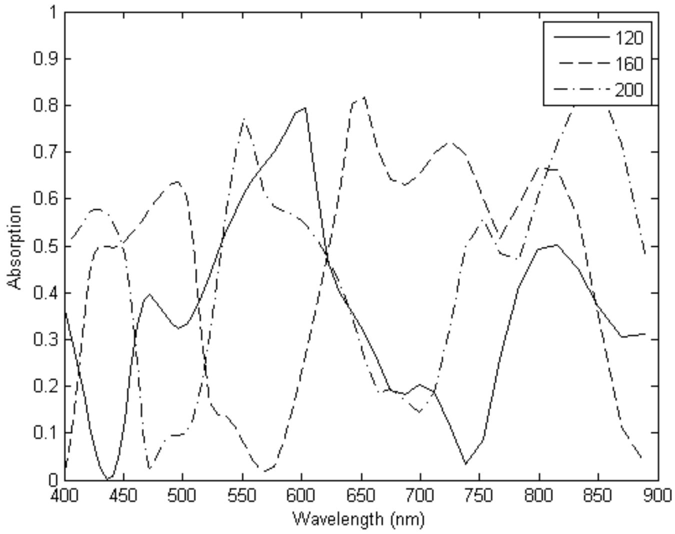

Fig. 4 – Computed absorption spectra of strip waveguide *versus* the operating wavelength for GaAs absorbing materials for different values of $d_2 = 120$, 160, and 200 nm.

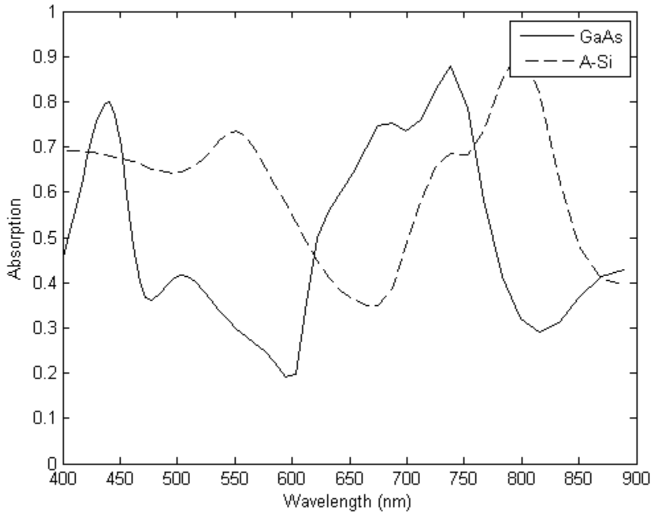

Fig. 5 – Computed absorption spectra of strip waveguide structure *versus* the operating wavelength for two different materials a-Si and GaAs for $d_2 = 120$ nm.

4. CONCLUSION

In this work, we investigated the light trapping in two materials used in a specific complex waveguide structure, namely, GaAs and a-Si. A novel software code based on the FDTD method has been devised and implemented to compute the reflectance, transmittance, and absorption spectra of the proposed complex waveguide structure model. The present study shows that the GaAs is still a promising candidate for light trapping and could be used in future potential applications in solar cell technology. The reflectance, transmittance, and absorption spectra exhibit interference patterns due to multiple reflection of light through the waveguide structure. In future works we plan to investigate the characteristic effects of the whole solar cell model based on the considered waveguide structure.

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