THE EFFECTS OF EMBEDDING MEDIUM AND SIZES ON THE OPTICAL ABSORPTION IN VERTICALLY ALIGNED GaAs NANOWIRES ARRAY BASED PHOTOVOLTAIC SOLAR CELLS

[1]R.M. DE LA CRUZ, [2]C. KANYINDA-MALU, [1]J.E. MUÑOZ SANTIUSTE, [1]E. SALAS,
[1]E. GARCÍA-TABARÉS, [1]M. TARDÍO, [1]S. ATHANASOPOULOS, [1]B. GALIANA

[1]University Carlos III of Madrid, Leganés (Madrid), Spain, EU, rmc@fis.uc3m.es

[2]University Rey Juan Carlos, FCSJ, Madrid, Spain, EU, clement.kanyindamalu@urjc.es

https://doi.org/10.37904/nanocon.2022.4580

Abstract

We theoretically investigate the effects of the surrounding media and sizes on the optical absorbance of a periodic square array of GaAs nanowires (NWs) as a candidate of photovoltaic solar cells. The filling media considered are: PMMA, Polycarbonate, Polystyrene and PVP, commonly used in the science and technology of semiconductors. The sizes considered are the NWs length and radius and the pitch array. The simulated system consists of a top layer of ITO, the active layer of GaAs NWs surrounded by an embedding medium and a substrate layer of Si. The system absorbance is modelled though the transfer matrix method; while the GaAs NWs with the embedding medium is considered as an effective medium modelled by Maxwell-Garnett theory. For s- and p-polarization, we find that the embedding medium effects on the absorbance spectra are scarcely perceptible compared with the size effects. Indeed, for longer and wider NWs and smaller pitches array, the absorbance values are greater around 600-1100 nm. These results are in good agreement with those reported in the literature by experiments and other sophisticated simulations in III-V semiconductor NWs.

Keywords: Absorption spectra, GaAs NWs array, Solar cells, Transfer matrix method, Maxwell-Garnett theory

1. INTRODUCTION

Nowadays, the research on gallium arsenide (GaAs) nanowires (NWs) is gaining an increasing interest due to their relevant applications in different fields, specifically in photovoltaics solar cells [1]. Indeed, the NWs material has exciting absorption characteristics because of their geometry [2], giving them exceptional light interaction features, not found in a bulk material, as consequence of their large aspect ratio. Increasing the absorption of light in GaAs NWs based solar cells is crucial to enhance the overall efficiency and reducing cost. Two main aspects to investigate in order to improve the light absorption in GaAs NWs can be the embedding medium of NWs and their sizes (NWs length and radius and pitch array).

Floris et al. [2] investigated the optical reflectance of InAs NWs for different filling media. In addition, several authors investigated experimentally and theoretically the sizes dependence on the optical spectra in semiconductor NWs array based solar cells [3,4]. These authors used finite difference time domain (FDTD) method, which takes a long time of calculation. However, we recently investigated the geometrical parameters dependence on the optical reflectance of GaAs NWs array simulated by means of the transfer matrix formalism and effective medium theory, where the computing time of calculation is less than that of FDTD method [5]. In that work, we only simulated the optical reflectance and we neglected the substrate and top layer effects on the reflectance.

Therefore, we extend the previous work in order to investigate the embedding medium and sizes effects on the absorbance of a GaAs NWs array based photovoltaic solar cells to gain insight about the system efficiency. We also included the effect of the top layer and substrate. A better absorption entails a higher efficiency. We use the transfer matrix formalism to simulate the optical absorbance. To evaluate the dielectric function of the continuum medium (GaAs NWs+embedding material), we use the Maxwell-Garnett (M-G) theory [6].

2. INVESTIGATED SYSTEM AND THEORETICAL MODEL

Figure 1 depicts the scheme of the investigated system constituted by (1) a semi-infinite air space; (2) a layer of indium tin oxide (ITO), transparent in the VIS range and extensively used in solar cells technology, with dielectric function (ε_2) [7] and thickness d_2 = 100 nm; (3) the active layer based on effective medium of GaAs NWs embedded in insulator material, with thickness d_3 = h (NWs length) and dielectric function described later; (4) a layer of silicon (Si) as substrate, with dielectric constant $\varepsilon_4 = 17.749 + 0.50381\,i$ (value at 517 nm) [8] and thickness d_4 = 2000 nm and (5) a semi-infinite air space. The light is impinging from the air and is going out to the air, then $\varepsilon_1 = \varepsilon_5 = 1$. The election of the above thicknesses is taken with the objective of a better light trapping in the array and a better confinement of the GaAs NWs.

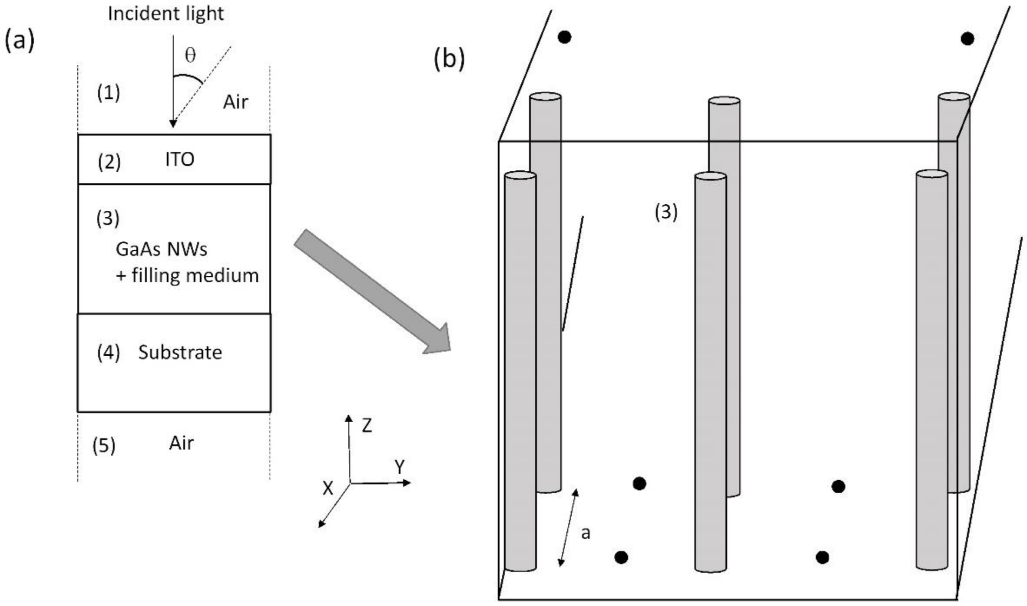

Figure 1 Scheme of the investigated system with the different layers (Figure 1a). Figure 1b is the zoom of the active layer (GaAs NWs+embedding medium). The black points represent the NWs array.

As embedding media, we chose PMMA, Polycarbonate, Polystyrene and PVP. Their dielectric function dependences on the wavelength are taken from ref. [8]. The array is characterized by cylinder radii ranging between R = 15 nm to 45 nm, length h = 500 nm and 1000 nm and pitch array a = 100 nm, 200 nm and 300 nm. These geometrical values yield filling factor ($f = \pi(R/a)^2$) belonging to the range between 0.018 to 0.196. The dielectric functions of the effective medium (GaAs embedded in insulator material) are characterized by $\varepsilon_3^{\parallel}(\omega)$ and $\varepsilon_3^{\perp}(\omega)$, being the effective dielectric functions in the directions parallel and perpendicular to the axis of cylindrical NWs, respectively. We use the M-G model under the assumption of a small inclusion density [6,9]; therefore

$$\varepsilon_3^{\parallel}(\omega) = f\,\varepsilon_{NW}(\omega) + (1 - f)\,\varepsilon_e \qquad (1)$$

where f is the filling factor, ε_e is the embedding material dielectric function and $\varepsilon_{NW}(\omega)$ is the GaAs NWs dielectric function that we will describe later. On the other hand, $\varepsilon_3^{\perp}(\omega)$ is written as [9]

$$\varepsilon_3^{\perp}(\omega) = \varepsilon_e\,[(\varepsilon_{NW}(\omega)(1 + f) + \varepsilon_e(1 - f))/(\varepsilon_{NW}(\omega)(1 - f) + \varepsilon_e(1 + f))] \qquad (2)$$

To describe $\varepsilon_{NW}(\omega)$, we use the formalism of Webb [10], where the exciton confinement energy is considered as a resonance. All parameters are extensively defined in ref. [10]. This formalism is appropriate for low-dimensional systems such as our NWs array.

With the knowledge of the dielectric permittivity of each layer, we use the transfer matrix method for our system constituted by five layers with four interfaces, similarly reported in ref. [11]. Then, the reflectance is $R^{(s,p)} = |r^{(s,p)}|^2$, where the superscripts s, p refer to s- and p- polarization, respectively; while the transmittance is $T^{(s,p)} = |t^{(s,p)}|^2$, being $r^{(s,p)}$ and $t^{(s,p)}$ the reflection and transmission coefficients, defined in ref. [11]. The absorbance of the stacked layer is defined as $A^{(s,p)} = 1 - R^{(s,p)} - T^{(s,p)}$. We implement the numerical simulations over the wavelength range 300 nm to 1100 nm, which cover the relevant parts of solar spectrum.

3. RESULTS AND DISCUSSION

To clarify the presentation of our results, we divide the discussion in two subsections, accounting for the effects of embedding material and the geometrical parameter sizes on the absorbance of GaAs NWs for s- and p-polarized light.

3.1. Embedding material effects on the absorbance of GaAs NWs

We show in **Figure 2a** the absorbance for the four investigated embedding media with fixed geometrical parameters (R = 25 nm, a = 200 nm and h = 500 nm) for s-polarized light at normal incidence. **Figure 2b** represents the comparison between s- and p-polarization at normal incidence when the insulator material is PMMA, as an example.

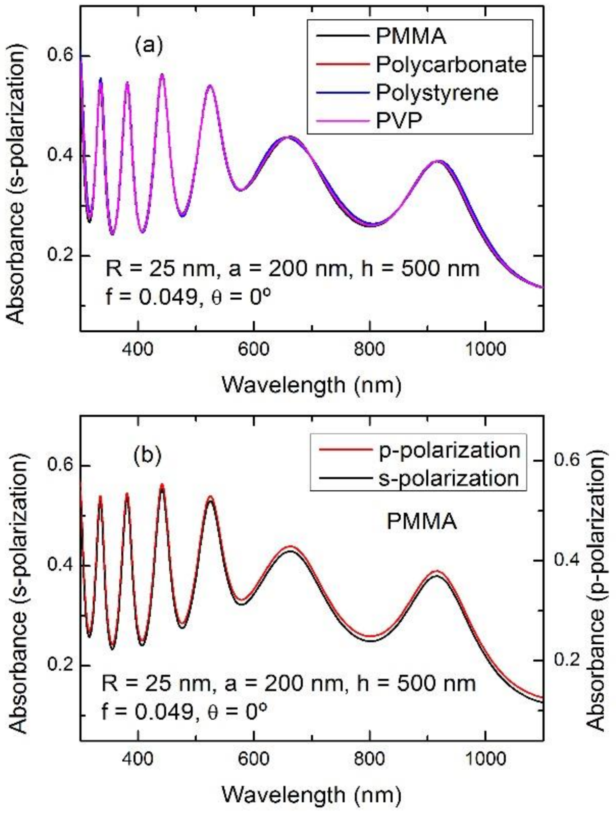

Figure 2 Absorbance for s-polarization of GaAs NWs surrounded by PMMA, Polycarbonate, Polystyrene and PVP at normal incidence (a). Absorbance for s- and p-polarization of GaAs NWs embedded in PMMA. In this figure, left and right axis are sligthly displaced to show both spectra (b).

We obtain an oscillatory behavior of the absorbance with the wavelength for all investigated embedding media for s- and p-polarization. This oscillatory behavior is typical in periodical systems [12] as a consequence of the interference effects; i.e., as light impinges on the NWs, photons can interact with NWs and undergo multiple scattering, yielding interference effects due to relative phase difference between reflected waves. The absorbance spectra for s- and p-polatization at normal incidence are identical. **Figure 2b** depicts the absorbance for both polarizations at normal incidence when the insulator material is PMMA, as an example. We previously obtained identical reflectance values for s- and p-polarization in GaAs NWs at normal incidence [5]. Sikdar et al. [11] also obtained reflectance spectra with identical reflection for both s- and p-polarized light at normal incidence for nanoparticles layers. On the other hand, the embedding medium effect in the absorbance is more significant in the range 600-800 nm, where there is a slight absorbance difference. The similar refractive indexes of the investigated polymers, appear to be the origin of the small embedding effect found in the absorption spectra of GaAs NWs. For the next section, we chose PMMA as filling medium in GaAs NWs to investigate the size effects.

3.2. Size effects on the absorbance of GaAs NWs

Figure 3 depicts the absorbance dependence on NWs length for s- and p-polarization at normal incidence with fixed R = 25 nm and a = 200 nm. The values of investigated length are h = 500 nm and 1000 nm.

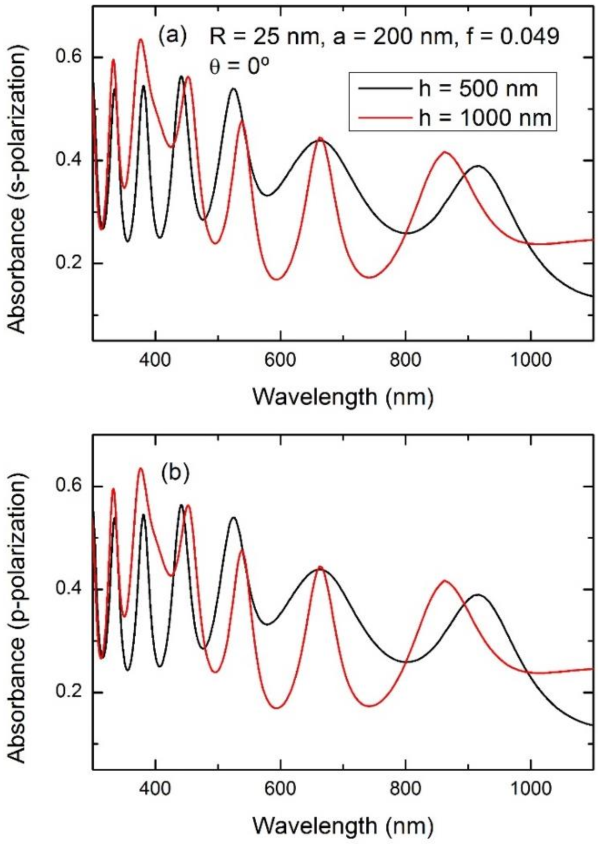

Figure 3 Absorbance for s-polarization (a) and p-polarization (b) of GaAs NWs embedded by PMMA with fixed R, a and f. The code of colors is the same for figures (a) and (b).

For both polarizations and lengths, we obtain again oscillatory behavior of the absorbance, typical of periodical systems. The absorbance is greater for h = 1000 nm in the range 300 nm to 500 nm. As the length changes, there is a difference in the phase factor; then, the absorbance values clearly depend on this geometrical parameter. Several authors showed experimentally and theoretically that the optical absorbance is greater for longer III-V semiconductor NWs [13]. Then, longer NWs benefit the light trapping in the array and consequently, the optical absorbance increases yielding a plausible gain efficiency in GaAs NWs photovoltaic solar cells.

We show in **Figure 4** the absorbance dependence on NWs radius for s- and p-polarization at normal incidence with fixed a = 200 nm and h = 500 nm. The investigated radii are R = 15 nm, 25 nm, 35 nm and 45 nm.

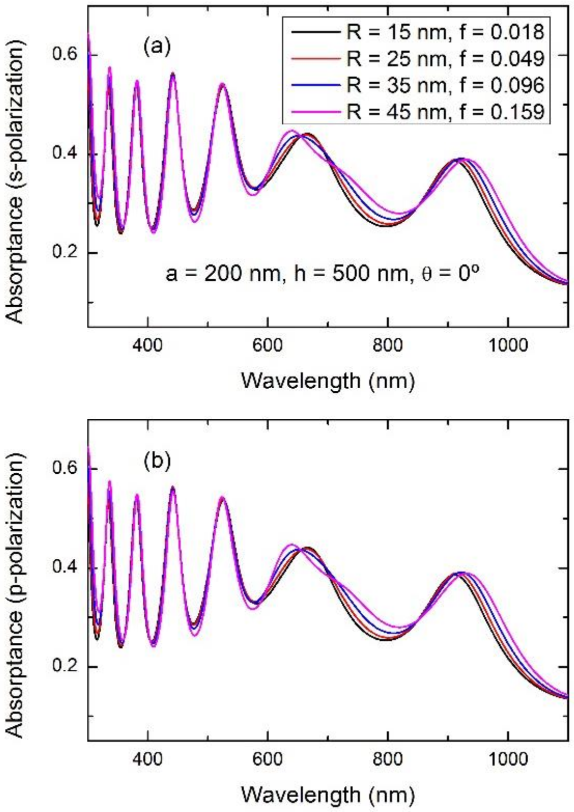

Figure 4 Absorbance for s-polarization (a) and p-polarization (b) of GaAs NWs embedded by PMMA with fixed a and h. The code of colors is the same for figures (a) and (b).

For increasing radius, our simulations show that the absorbance is slightly greater in the range 600 nm to 1100 nm. Ali et al. [14] theoretically showed that the absorption is greater for wider GaAs/GaSb NWs, in good agreement with our results. On the other hand, we obtain a red-shift of the absorbance modulations with increasing radius. Dhindsa et al. [3] previously reported this phenomenon for experimental and simulated reflectance by FDTD method in GaAs NWs array.

Although it is not shown here, for smaller pitch array, our simulations show greater absorbance values in the range 600 nm to 1100 nm, in good agreement with that reported by Dhindsa et al. [3] in GaAs NWs. A smaller pitch array entails a greater number of absorbance centers (greater filling factor), then the absorbance values should be greater.

4. CONCLUSION

We have calculated the embedding material and sizes effects on the optical absorbance of GaAs NWs array based photovoltaic solar cells. We simulated the absorbance spectra using the transfer matrix formalism and Maxwell-Garnett model. An oscillatory behavior of the absorbance for s- and p-polarized light, independently of the embedding medium and sizes, is found. We investigated as embedding media PMMA, Polycarbonate, Polystyrene and PVP, commonly used in the science and technology of semiconductors. We have found that for both polarizations, the embedding medium effects on the absorbance are scarcely perceptible compared with the sizes effects. Indeed, for longer and wider NWs and smaller pitches array, the absorbance values are greater in the range 600-1100 nm. These numerical results are in good agreement with those reported in the literature by experiments and sophisticated FDTD simulations in III-V semiconductor NWs.

ACKNOWLEDGEMENTS

This work was partially supported by Spanish MICINN under grant RTI 2018-101020-B-I00 and TECHNOFUSION III CM-S2018IEMAT-4437. This work has also been supported by Comunidad de Madrid under the agreement with UC3M in the line of Excellence of University Professors (EPUC3M14).

REFERENCES

[1] MARIANI, G., SCOFIELD, A.C., HUNG, C.-H., HUFFAKER, D.L. GaAs nanopillar-array solar cells employed in situ surface passivation. *Nat. Commun*. 2013, vol. 4, no. 1497, p. 7.

[2] FLORIS, F., FORNASARI, L., MARINI, A., BELLANI, V., BANFI, F., RODDARO, S., ERCOLANI, D., ROCCI, M., BELTRAM, F., CECCHINI, M., SORBA, L., ROSSELLA, F. Self-assembled InAs nanowires as optical reflectors. *Nanomaterials.* 2017, vol. 7, no. 400, p. 11.

[3] DHINDSA, N., CHIA, A., BOULANGER, J., KHODADAD, I., LAPIERRE, R., SAINI, S.S. Highly ordered vertical GaAs nanowire arrays with dry etching and their optical properties. *Nanotechnology.* 2014, vol. 25, 305303, p. 11.

[4] AZIZUR-RAHMANAND, K.M., LAPIERRE, R.R. Wavelength-selective absorptance in GaAs, InP and InAs nanowire arrays. *Nanotechnology.* 2015, vol. 26, 295202, p. 7.

[5] DE LA CRUZ, R.M., KANYINDA-MALU, C., MUÑOZ SANTIUSTE, J.E. Simulations of optical reflectance invertically aligned GaAs nanowires array: The effect of the geometrical structural parameter. *Physica B.* 2022, vol. 639, 41393, p. 7.

[6] MAXWELL-GARNETT, J.C. Colours in Metal Glasses and in Metallic Films. *Trans. Of the Royal Society.* 1904, vol. CCIII, pp 385-420.

[7] KORNYSHEV, A.A., MARINESCU, M., PAGET, J., URBAKH, M. Reflection of light by metal nanoparticles at electrodes. *Phys. Chem. Chem. Phys.* 2012, vol. 14, pp 1850-1859.

[8] RefractiveIndex.INFO. Refractive index database [online] 2022. [viewed 2022-07-30]. Available from: https://refractiveindex.info/?shelf=3dbook=plasticspage.

[9] STARKO-BOWES, R., ATKINSON, J., NEWMAN, H., HU, T., KALLOS, T., PALIKARAS, G., FEDOSEJEVS, R., PRAMANIK, S., JACOB, Z. Optical characterization of epsilon-near-zero pole, and hyperbolic response in nanowire metamaterials. *J. of the Optical Society of America B.* 2015, vol. 32, pp 2074-2080.

[10] WEBB, K.J., LUDWIG, A. Semiconductor quantum dot mixture as a lossless negative dielectric constant optical material. *Phys. Rev. B* 2008, vol. 78, 153303, p. 4.

[11] SIKDAR, D., KORNYSHEV, A.A. Theory of tailorable optical response of two-dimensional arrays of plasmonic nanoparticles at dielectric interfaces. *Scientific Reports.* 2016, 33712, p. 6.

[12] CHEN, Y, HÖHN, O., TUCHER, N., PISTOL, M.-E., ANTTU, N. Optical analysis of a III-V-nanowire-array-on-Si dual junction solar cell. *Optics Express.* 2017, vol. 25, A665, p. 15.

[13] DHINDSA, N., KOANDHANI, R., SAINIA, S.S. Length dependent optical characteristics analysis for semiconductor nanowires. *Nanotechnology.* 2020, vol. 31, 224001, p. 9.

[14] ALI, L.M., ABED, F.A. Numerical modeling of opto-electric characterization of GaAs/GaSb nanowire solar cells. *Optical and Quantum Electronics*. 2020, vol. 52, no. 154, p. 9.