Optimization of Solar Cells with Various Shaped Surficial Nanostructures

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***Abstract*— In this paper, the effect of different surficial nanostructure designs on the absorption efficiency of thin film GaAs solar cells is investigated numerically. For this, six surficial photonic nanostructures over a GaAs substrate have been applied and the optical properties are observed including reflectance, transmittance, and absorption. Two optimized surficial structures which have higher efficiency are used on a fundamental PN junction GaAs solar cell and the efficiency enhancement are observed along with some other electrical properties including open circuit voltage, short circuit current, and maximum power point. Current at maximum power point ware improved from 1.69 to 1.84 mA, the voltage at the maximum power point decreased by 0.02 volts. The fill factor is improved around 3% and the maximum efficiency is increased by around 1.24%. This work gives a clear idea of the possible techniques for applying surficial nanostructures for photon management and improving the thin-film GaAs solar cell efficiency.**

Keywords* — *Solar cells, nanoholes, nanostructures, square gratings, light trapping.

1. Introduction

Global energy demand is increasing very fast as the population increases rapidly. Fossil fuels are limited in nature, expensive, and harmful to the environment. Researchers are trying to find the best alternative renewable energy to fulfill the growing energy demands. Solar energy is one of the promising renewable energies as its availability throughout the world and it is free of cost. Earth receives 10,000 times more solar energy than the energy it consumes in a year [1]. A recent trend of research is to design solar cells to convert photon energy to electrical energy efficiently at low cost.

Over the last few decades, researchers have been investigating different structures and technologies to obtain highly efficient solar cells. Among all the techniques, increasing photon absorption by light trapping is the significant one. Nanoholes over Si wafers have been fabricated by the combination of deep ultraviolet lithography (UVL) and metal-assisted Si etching in aqueous oxidizing hydrofluoric acid (HF) [2]. Periodic and random nanoholes have been investigated to increase light trapping on Si solar cells [3] and GaAs solar cells [4] where absorption has been increased from 70% to 110%. 60%-96% average absorption found in the 550nm thick Si solar cell containing cluster nanohole array [5]. Pyramid shaped surficial nanostructures have been considered in [6] to fabricate multiple absorption and reflection on a set of textured surfaces. Nanocones and nanowires surficial structures have been treated as one of the mechanisms as these geometries improve light absorption by increasing effective surface area, decreasing reflection, and improving the path length of the photon [7]. Kinked short nanowire array containing total length of 1–1.5 μm exhibit remarkable efficiency exceeding 14% [8]. The kinked morphology increases optical path, exciting more resonance modes, and reducing the transmission into the substrate which all lead to increase the absorption. Light harvesting by nano-honeycomb surficial structures has been applied in [9-10] to improve light trapping ability and reducing the thickness of the active material needed for absorption. Rectangular and square gratings are notable nanostructure designs that have been experimented with as the design improves light trapping ability and induces a plasmonic effect [11-12]. The design enhances the light-matter interaction more than a flat surface or bare substrate due to its uneven surficial structure.

In this article, thin-film GaAs solar cells containing different surficial structures have been designed and compared with bare GaAs substrate. The reflectance, transmittance, and absorption spectra are calculated numerically using the Finite Difference Time Domain (FDTD) method. It is found that the reflectance of all geometry is less than the bare substrate. Hence, the absorption of light at surficial nanostructures is more excellent. The comparison between different surficial structures will provide an idea of light scattering over the solar cell surface and will help to choose optimized highly efficient solar cells.

2. Methodology

The geometries are constructed and the absorption profile is calculated numerically by ANSYS Lumerical FDTD Solution [13]. The software is for modeling nanophotonic devices, processes, and materials. It provides an integrated design environment for scripting ability, post-processing, and optimization routine.

2.1. Optical Simulation Setup

A rectangular-shaped GaAs substrate was placed on a 3D FDTD simulation region. The thickness of the substrate was considered 1.7 μm [14]. The simulation temperature was set to 300 °K and perfectly matched layers (PML) were used as boundary conditions. A plane wave source was placed over the substrate but situated inside the simulation region.

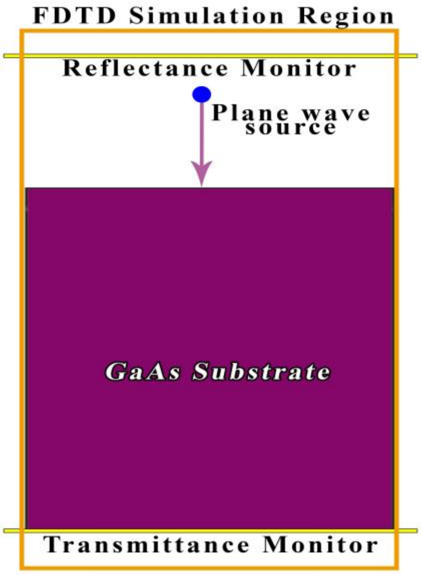


Fig. 1: Optical simulation set up for obtaining absorption profile

The wavelength of the plane wave source laid between 0.4 µm to 0.8 µm which is the visible wavelength range. Two power monitors were placed inside the simulation region to calculate the reflectance and transmittance. Absorption was calculated from the source to the reflectance and transmittance. Nanostructures were placed at the top surface of the substrate.

Figure 1 shows the simulation setup of Lumerical FDTD for a bare GaAs substrate where two monitors and their position were visible. The same setup along with surficial nanoholes or nanostructures were also investigated.

2.2. Design of Surficial Nanoholes or Nanostructures

Fig. 2 shows the different surficial nanostructures used to improve solar cell performance. They are described in brief in the following sections.

- **Circular nanoholes:** Circular nanoholes reduce the surface area of solar cells. Thus, the reflection of light also decreases which leads to improve light absorption. Thinner and flexible solar cells could be designed using circular nanoholes. Periodic circular nanoholes are applied over the surface of the GaAs substrate. The radius of the circles is 50 nm and the z span or depth of the circles is 50 nm. The nanoholes are empty or filled with air.

- **Hexagonal nanoholes:** Hexagonal nanoholes or honeycomb nanoholes increase light absorption of solar cell by improving light trapping capability. The nanoholes increase surface area, reduce reflection, and increase flexibility. In this case, periodic hexagonal nanoholes were considered. Each side of the hexagon is 50 nm long. The z span or depth of the hexagon is also 50 nm. The nanoholes are remains empty or filled with air.

- **Rectangular nanostructures and square gratings:** The rectangular nanostructure and square gratings design creates a linear pattern over the solar cell surface. The pattern helps to reduce reflection and increases the surface area. Hence absorption improves. The dimension of the rectangles are 100 nm width and 50 nm height and the square gratings are 50 nm width and 50 nm height.

- **TiO_2 nano pyramid:** The structure in this simulation contains a TiO_2 pyramid pattern to enhance the optical performance. The pattern acts like an anti-reflecting coating. This reduces surface recombination by minimizing the surface area of the solar cell. The TiO_2 pyramid geometry can enhance photocatalytic activity and make the structure more efficient in absorbing light for energy conversion. Also, the sharp tips of the pyramid can enhance the localized electric field.

- **Nanocone:** Surficial nanocones can improve the efficiency of solar cells by increasing surface area, improving light trapping capability, increasing internal reflection inside the nanoholes, and reducing reflection losses. In simulation, 50 nm top radius and 50 nm z span or depth of the nanocone have been considered. The nanocones are arranged in a periodic manner.

3. Results and discussion

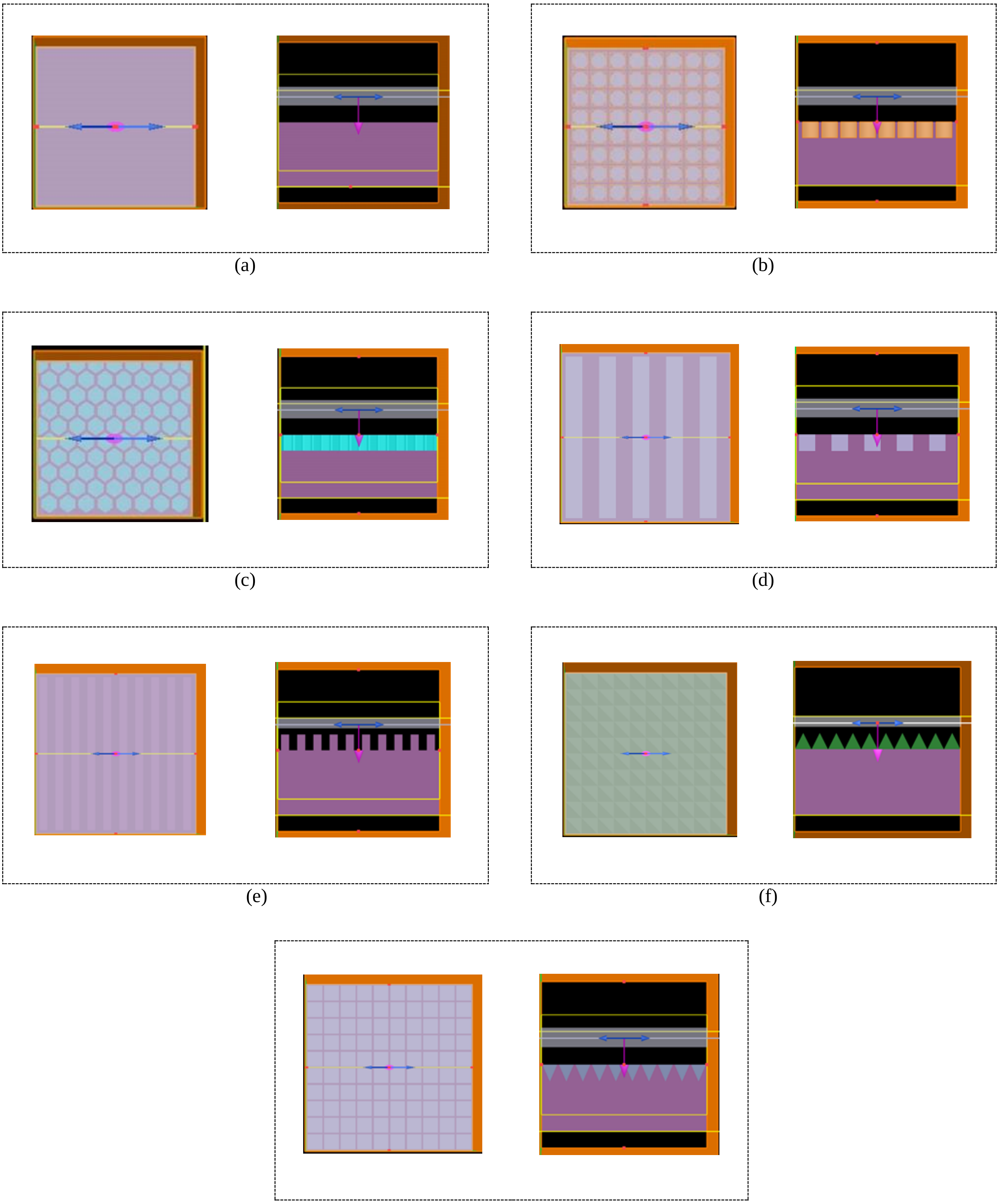
After the suitable simulation setup and boundary conditions, the simulation is conducted and the required data for visualizing characteristics are collected using FDTD solver. The design which has highest light-absorbing capability is further investigated for electrical simulation on the Ansys Lumerical Charge solver.

3.1 Optical Results

Fig. 3 shows the reflectance of the incident plane wave over bare GaAs substrate and different surficial nanostructure designs. The graph represents the reflectance of visible wavelength which usually lies between 0.4 µm to 0.8 µm. From the graph, it is clearly visible that, the reflectance of about all surficial nanostructure designs is less than the reflectance of bare GaAs substrate. Among all surficial nanostructure designs, the reflectance of square gratings and circular nanoholes are less than the other designs for all over the spectrum.

The transmittance graph shown in Fig. 4, represents that all surficial nanostructure designs have more transmittance than the bare substrate. Hexagonal nanoholes and circular nanoholes allow more light to transmit over the substrate compared to the other designs.

It is clearly visible from the absorption graph shown in Fig. 5 that, the surficial nanostructures increase the light absorption as compared to the bare GaAs substrate. The light absorption of about all surficial nanostructures is above that of the bare substrate. The nanocone, TiO_2 nanopyramid, hexagonal nanoholes, and rectangular nanostructures are the design that improves light absorption but square gratings and circular nanoholes absorb the highest amount. These two designs have been considered for future electrical stimulation.



(a) (b) (c) (d) (e) (f) (g)

Fig. 2: Top and side view of (a) bare GaAs substrate, (b) circular nanoholes, (c) hexagonal nanoholes, (d) rectangular nanostructures, (e) square gratings, (f) TiO2 nanopyramid and (g) nanocone surficial nanostructure designs.

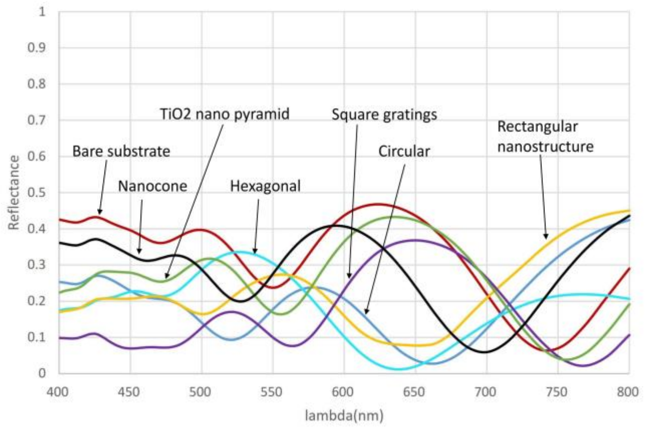


Fig. 3: Reflectance profile of bare GaAs substrate and different surficial nanostructures/nanoholes design

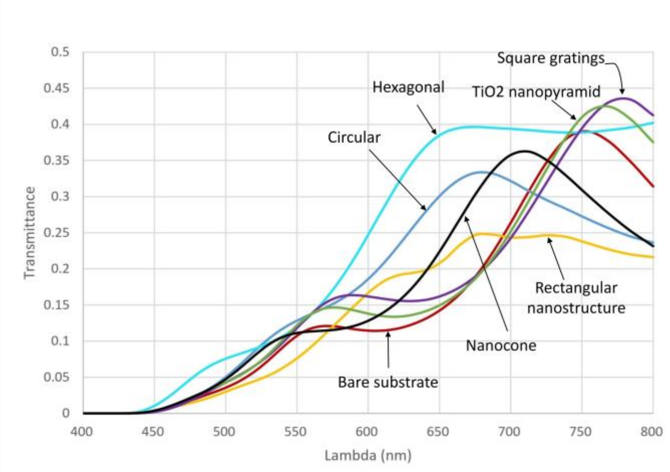


Fig. 4: Transmittance profile of bare GaAs substrate and different surficial nanostructures/nanoholes design

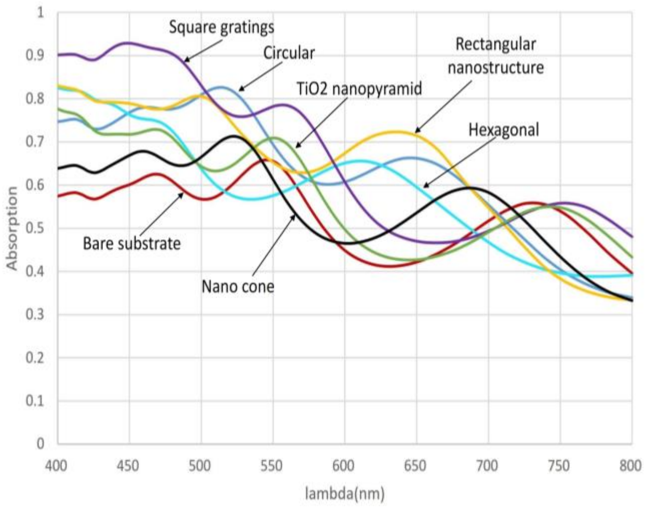
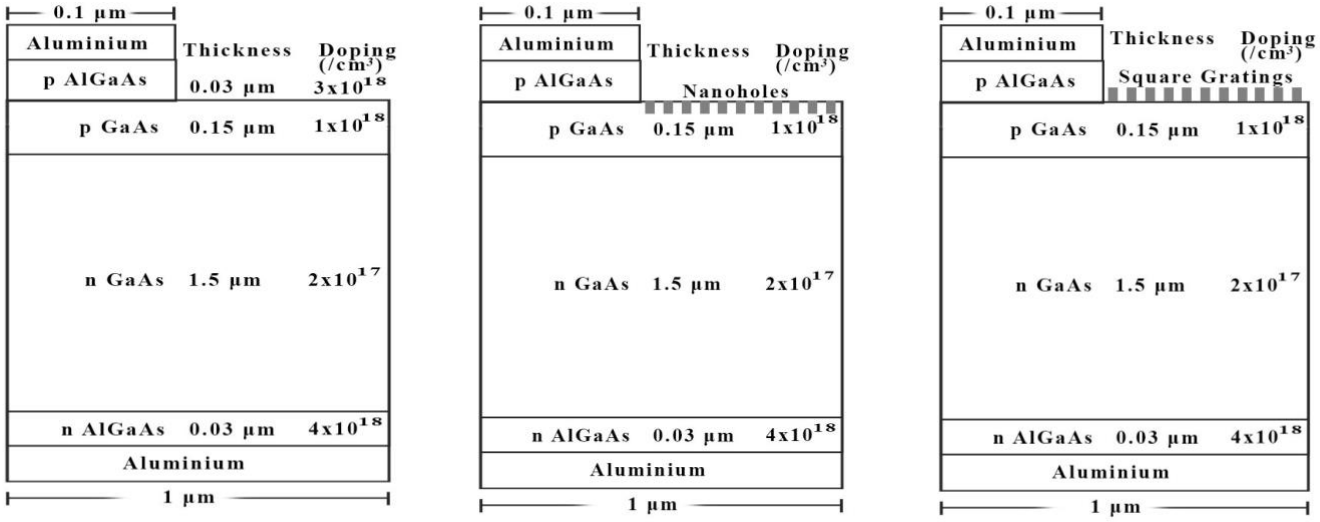


Fig. 5: Absorption profile of bare GaAs substrate and different surficial nanostructures/nanoholes design.

3.2. Electrical Simulation Results

Ansys Lumerical Charge solver is used for the electrical simulation. The simulation setup including doping concentrations and dimensions, different recombination rates, contact resistances, etc. are considered from [14]. Two heterojunction layers are created between the front and back contact to the substrate for career collection.

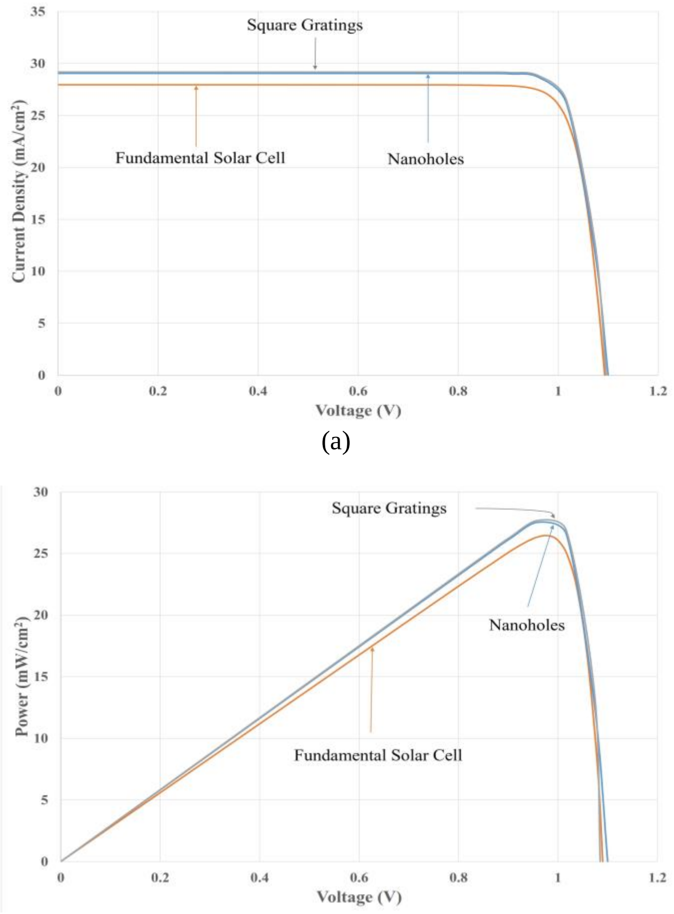
Different structures created for electrical simulation are shown in Fig. 6. Fig. 6(a) represents a fundamental P-N junction solar cell without any surficial structure or nanoholes. Fig. 6(b) is the solar cell with circular nanoholes and Fig. 6(c) is the solar cell with square gratings over the surface.



(a) (b) (c)

Fig. 6: Electrical simulation setup for (a) fundamental P-N junction solar cell, (b) solar cell with circular nanoholes,(c) solar cell with square gratings.

The electrical characteristics J-V curve obtained from the simulation of the square gratings and the circular nanoholes are shown in Fig. 7(a) and P-V curves are shown in Fig. 7(b). The different electrical parameters obtained from simulation are shown in Table I.



(a)

(b)

Fig. 7: (a) J-V curve and (b) P-V curves of different solar cell

TABLE I. SOLAR CELL ELECTRICAL CHARACTERSTICS

Solar Cell Type	Voc (V)	Jsc (mA/cm^2)	Vmp (V)	Imp (mA)	FF	Max. η (%)
Fundamental PN junction solar cell	1.093	28.955	0.98	26.99	0.84	26.45
Nanoholes Arrangement	1.100	29.053	0.96	28.68	0.86	27.54
Square Grating Arrangement	1.096	29.183	0.96	28.83	0.87	27.69

The performance of the square grating arrangement of the present work has been compared with some other published work given in Table II. From the table it is clear that the present work improves the maximum efficiency of the solar cell.

TABLE II. PERFORMANCE COMPARISON TO DIFFERENT SOLAR CELLS

Ref.	Substrate material	Surficial design	Voc (V)	Jsc (mA/cm^2)	Max. η (%)
[2]	Si	Nanohole	0.566	32.2	9.51
[4]	GaAs	Nanohole	1.019	20.1	16.83
[7]	Si	Nanocone/ nanopillar	0.531	33.7	12.20
[9]	InGaN	SiO_2 nano-honeycomb	1.9	0.84	0.51
[13]	GaAs	Bare substrate	1.1	29.0	27.50
This work	GaAs	Square Grating	1.096	29.183	27.69

4. Conclusion

Six different nanoholes or surficial nanostructures have been applied on a GaAs solar cell and the light absorption for each design has been measured. It is found that the circular nanoholes and square gratings are the most efficient design among all the experimented designs. These two designs have been implemented over a fundamental P-N junction solar cell and the electrical characteristics have been observed. Open circuit voltage and short circuit current density were improved by using the surficial structures. Current at maximum power point improved from 1.69 to 1.84 mA. However, the voltage at the maximum power point decreased by 0.02 volts. The fill factor improved around 3% and the maximum efficiency increased by around 1.24%. Although the performance enhancement is not very high, still the techniques can be considered with other technologies to boost up the performance. Nanoholes or nanostructures with III-V material Multiple Quantum Well Solar Cell (MQWSC) could be another choice for further investigation.

References

[1] J. N. Ding, F. Q. Zhang, N. Y. Yuan, G. G. Cheng and X. Q. Wang. “A novel square silicon nanohole structure: Fabrication and antireflective property," International Conference on Materials for Renewable Energy and Environment, Vol. 1, pp. 85-88, 2013.

[2] K. Q. Peng, X. Wang, L. Li, X. L. Wu and S. T. Lee, “High-performance silicon nanohole solar cells,” Journal of American Chemical Society, Vol. 132, No. 20, pp. 6872–6873, 2010.

[3] F. Pratesi, M. Burresi, F. Riboli, K. Vynck and D. S. Wiersma, “Disordered photonic structures for light harvesting in solar cells,” Optics express, Vo. 21, Issue S3, pp. A460-A468, 2013.

[4] D. J. Paul, “Performance enhancement of iii-v multiple-quantum-well photovoltaic devices employing light harvesting nanohole assembly,” MSc. Engg. Thesis, Department of EEE, Bangladesh University of Engineering & Technology (BUET), Dhaka, Bangladesh, Aug. 2020.

[5] Moeini, S., Abdi, G., Bahador, H. et al. High-Performance a-Si Clustering Nanohole Arrays for Solar Photovoltaics. Silicon 15, 3497–3505 (2023). https://doi.org/10.1007/s12633-022-02276-4

[6] M. Rosa, M. Allegrezza, M. Canino, C. Summonte and A. Desalvo, “TMAH-textured, a-Si/c-Si, heterojunction solar cells with 10% reflectance,” Solar Energy Materials and Solar Cells, Vol. 95, No. 11, pp. 2987-2993, 2011.

[7] J. He, Z. Yang, P. Liu, S. Wu, P. Gao, M. Wang, S. Zhou, X. Li, H. Cao and J. Ye, “Enhanced electro-optical properties of nanocone/nanopillar dual-structured arrays for ultrathin silicon/organic hybrid solar cell applications,” Advanced Energy Materials, Vol. 6, Issue 8, 2016.

[8] Xin Yan, Peipei Xu, Yi Li, Xia Zhang, Xiaomin Ren “Enhanced light absorption of kinked nanowire arrays for high-performance solar cells,” Optics Communications, Volume 527, 2023, 128991, ISSN 0030-4018, https://doi.org/10.1016/j.optcom.2022.128991.

[9] J. Xavier and C. Becker, “Computational analysis of triangular and honeycomb lattice-structured tapered nanoholes for enhanced light trapping in thin-film Si solar cells,” Photonics for Solar Energy Systems V, Vol. 9140, 2014.

[10] P. H. Fu, G. J. Lin, C. H. Ho, C. A. Lin, C. F. Kang, Y. L. Lai, K. Y. Lai, and J. H. He, “Efficiency enhancement of InGaN multi-quantum-well solar cells via light-harvesting SiO2 nano-honeycombs,” Applied Physics Letters, Vol. 100, No. 1, 2012.

[11] T. K. Chong, J. Wilson, S. Mokkapati and K. R. Catchpole, “Optimal wavelength scale diffraction gratings for light trapping in solar cells,” Journal of Optics, Vo. 14, No. 2, 2012.

[12] H. Heidarzadeh, “Incident light management in a thin silicon solar cell using a two-dimensional grating according a Gaussian distribution,” Solar Energy, Vol. 189, pp. 457-463, 2019.

[13] Lumerical. [Online]. Available: https://www.lumerical.com/

[14] X. Wang, M. R. Khan, J. L. Gray, M. A. Alam and M. S. Lundstrom, “Design of GaAs solar cells operating close to the Shockley–Queisser limit,” IEEE Journal of Photovoltaics, Vol. 3, No. 2, pp. 737-744, 2013.