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In-Search of Efficient Anti-Reflection Coating Layer for Crystalline Silicon Solar Cells: Optimization of the Thickness of Niobium Pentoxide Thin Layer

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Abstract

The purpose of providing an anti-reflection coating (ARC) layer on the surface of crystalline silicon (c-Si) solar cells is to stipulate a unique dielectric material medium that causes destructive interference of the reflected light from device surfaces and minimizes the reflection of light. In this work, the thickness optimization of niobium pentoxide (Nb_2O_5) as an ARC layer for the high photovoltaic performance of the c-Si solar cell was carried out by a low-cost, sol-gel spin coating deposition process and further experimental results were validated by a personal computer one dimensional (PC1D) simulation study. The lowest average reflectance of ~7.21% was achieved at 75 nm thickness of the ARC layer as compared to other samples. For the simulation study, the different thicknesses of ARC layers were selected as input parameters to explore the photovoltaic characteristics of c-Si solar cells. The simulated results showed that the highest power conversion efficiency (PCE) of 17.92% and over 95% external quantum efficiency (EQE) were achieved with a 75 nm thickness of ARC layer-based c-Si solar cell. This work on the thickness optimization of the ARC layer would provide useful information to develop low-cost high-performance c-Si solar cells.

Keywords: Silicon solar cell; ARC layer; Nb_2O_5; Optimization; Thickness; Photovoltaic properties.
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1. Introduction

The important aspect in enriching the efficiency of solar cells is to reduce the reflection of solar radiation by providing an anti-reflection coating (ARC) layer on the top surface of the solar cell.[1-3] The ARC layer supports trapping the photons and pushing towards the p-n junction for the generation of high photocurrent.[4] The ARC materials having a higher absorption capability of incident light in the larger wavelength range would be appropriate for the application of solar cells.[5-7] Various ARC materials with a high refractive index like Si_3N_4, SiO_2–TiO_2, a-SiN_x, Ta_2O_5, MgF_2, ZnS, SiO, SiO_2, and TiO_2 have been already used in the fabrication of the c-Si solar cells.[8-10] For better efficiency of the solar cell, essentially it is to explore the promising ARC material leading to enhance the performance of solar cells. The ARC layer deposition technique can be appropriate for uniform layer deposition, which can also boost the efficiency of the cell.[11] The thickness of the ARC layer has a crucial role in trapping the wider spectrum of solar radiation for better performance of the solar cell.

Niobium Pentoxide (Nb_2O_5) is an n-type semiconductor with a bandgap of 3.4 eV and its remarkable physicochemical characteristics and structural isotropy make it appropriate for a wide range of applications in photoelectrodes as well as microelectronics devices.[12] Nb_2O_5 exhibits a high potential for application in solar cells because of its excellent stability in an aqueous medium. The properties like photocatalytic characteristics, redox, and surface acidity are intrinsically linked to its structure.[13] Nb_2O_5 is found abundantly in nature with high resistive power for corrosion and it is also thermodynamically stable. The thin films and nanostructured Nb_2O_5 have already been applied in batteries, solar cells, and

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other electronic devices such as memristors.[14] Nb_2O_5 is the most thermodynamically stable and forms minimum heat energy in comparison to other niobium oxides, such as NbO, and NbO_2.[15,16] Interestingly, Nb_2O_5 shows a highly stable oxidation number and an excellent transparent dielectric medium.[17] Nb_2O_5 films have exceptional chemical and physical characteristics like good absorption behavior of light, posing a high refractive index, and good chemical stability in any medium.[18-21] Nb_2O_5 as photoanode material has been drawing significant research interest due to its higher conduction band energy level than traditional TiO_2 and thus in principle produces higher open-circuit voltage and comparable electron injection efficiency as well as better chemical stability.[22] The high-quality thin film deposition of Nb_2O_5 is possible through simple and low-cost techniques like sol-gel spin-coating or dip-coating. It does not need high temperatures during the deposition of thin film as well as post-deposition treatment, which is an extra benefit to reduce the fabrication cost and it also supports the deposition of films onto heat-sensitive substrates.[23,24]

Macco *et al.* deposited a thin film of Nb_2O_5 layer by atomic layer deposition (ALD) and exhibited exciting passivating contact properties such as surface passivation, contact resistivity, and optical transparency in the field of the solar cell. High energy conversion efficiencies for crystalline silicon (c-Si) solar cells have been demonstrated using metal oxide passivating connections with low processing complexity.[25] Fernandes *et al.* deposited a thin layer of Nb_2O_5 and increased the conductivity by reducing the flow rate of oxygen due to inducing oxygen vacancies, leading to solar cells with better efficiency.[14] In 2019, Afzali, *et al*. simulated by using analysis of microelectronic and photonic structures one-dimensional (AMPS1-D) software and PV properties of amorphous silicon solar cells. By deposing an 80 nm thick Nb_2O_5 layer as transparent conducting oxide (TCO) layer on the surface of the cell, the value of open-circuit voltage, efficiency, and the fill factor increase dramatically, and the efficiency of the cell increases from 8.2% to 10.9%.[18]

In this work, a sol-gel-derived precursor of Nb_2O_5 is deposited on the silicon substrate by spin-coating technique at different spinning rates, and the thickness of the layer is optimized by ultraviolet diffuse reflectance spectroscopy (UV-DRS) spectroscopy. Furthermore, the PC1D simulation software was applied for the characterization of PV properties and the simulated results have shown that the highest PCE of 17.92% and more than 95% EQE at 75 nm thickness of the ARC layer, which might be efficient for c-Si solar cells.

2. Material and experimental method

2.1 Preparation of precursor and deposition of ARC layers

A niobium-precursor was prepared by dissolving 0.4 g of niobium(V) chloride ($NbCl_5$, Aldrich, 99%) in 8.5 ml of ethanol (99%, Sigma-Aldrich) and 0.2 ml of deionized (DI) water under vigorous stirring of 1 h and placed for 48 h at laboratory conditions before deposition by spin-coating. A highly transparent and stable solution was obtained without any other additives. A p-type c-Si substrate of area 16 cm^2, of thickness 200 μm, and sheet resistance 1–3 $\Omega/\square$ was selected. A uniform textured silicon substrate was obtained by fully dipping in an alkaline solution containing 2% KOH, 2% TCS-40, and DI water for 15–20 min at 80 °C. After cleaning with DI water for 20 minutes by sonication, the phosphorous diffusion was conducted by retaining the textured substrate in the quartz boat and placed in a horizontally fixed quartz diffusion furnace followed by injecting 1200 sccm phosphoryl chloride ($POCl_3$) gas into the furnace at 800 °C. After n-layer P diffusion, the substrate was designated as an n-p-n structure and possessed surface resistances of ~70 $\Omega/\square$ on both sides. Phosphorous glass (PSG) was taken out from the n-p-n substrate's surface by using a 5% hydrofluoric acid (HF) solution. After that, a thin Nb_2O_5 film was deposited by dropping 0.2 ml prepared precursor on the n-p-n substrate and spinning them at a different rates of 1000, 2000, and 3000 rpm for 30 s and immediately dried at 70 °C for 15 min in the oven. The schematic diagram ARC layer-based c-Si solar cell is depicted in (Fig. 1). The deposited films were calcinated in the air at different temperatures in two steps, in the first step, it was annealed at 100 °C for 1 h and in the second step, it was annealed at 500 °C for 2 h with 5 °C/min acceleration to remove impurities.

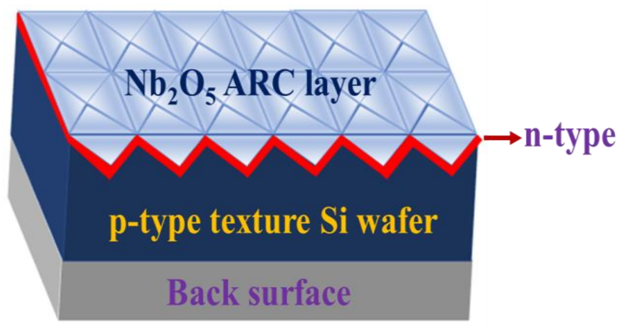

Fig. 1 Schematic diagram of Nb_2O_5 ARC layer-based c-Si solar cell.

2.2 Characterizations

The Nb_2O_5 layer deposited on the silicon substrate was characterized by different types of analytical, spectroscopic, and photovoltaic measurement techniques. The crystalline properties were examined by the Rigaku X-rays diffractometer with a Ni-filtered CuKα source. The crystalline structure and phase of Nb_2O_5 deposited over solar cells were examined by X-rays diffraction (XRD). For surface morphology, field emission scanning electron microscopy (FESEM, Hitachi 4800, Japan) was employed. The optical property such as the reflectance of the Nb_2O_5 layer deposited on Si was evaluated by ultraviolet-diffuse reflectance spectroscopy (UV-DRS, Shimadzu MPC-3100). The carrier lifetime mapping of the Nb_2O_5 layer deposited on Si was determined to analyze the bulk charge carrier lifetime and sheet resistance over the substrate's surface. The details of photovoltaic properties were revealed by PC1D simulation by using average reflectance and refractive index as input key parameters.

2.3 PC1D simulation

PC1D software is the best simulating tool using a finite-element numerical method for solving the coupled nonlinear equations for carrier generation, recombination, and transport in solar devices. It can be used both for the simulation of device performance and to understand the fundamentals of solar cell physics.[26] The main advantages of PC1D include the high calculation speed, spontaneous interface derivation, and extensive material and physical parameters.[27] A PC1D simulating tool was used for the simulation of PV characteristics of solar cells by taking the average reflectance, refractive index, and thickness of ARC layers as key input parameters. There are several simulation software for solar cells, such as PC1D, automat for simulation of heterostructures (AFORS-HET), AMPS-1D, and solar cell capacitance simulator (SCAPS).[28] PC1D was invented at Sandia National Laboratory and then further modified by the University of New South Wales, Australia.[29] PC1D allows to simulate of many characteristics of semiconductor devices, and it consists of several files of the refractive index, bandgap, electron affinity, dielectric constant, electron-hole motilities, carrier lifetimes, doping concentration, *etc.* for c-Si, a-Si, GaAs, Ge, InP, GIN, and AlGaAs based semiconductor devices.[30-32] The input data or parameters are summarized in Table 1 for the simulation study and performed by adopting the light irradiation having AM1.5 (0.1 W/cm^2) at 300 K temperature. The bulk recombination time was increased to 10 seconds, the p-type background doping concentration was increased to 1.153 × 10^{16} cm^{-3}, and the first front diffusion was increased to 2.87 × 10^{20} cm^{-3} for the simulation.[33]

Table 1. Inset of primary parameters used in the PC1D simulation program.

Parameters	Value
Device area	100 cm^2
Base layer thickness	150 μm
Emitter layer thickness	2 μm
The thickness of the Nb_2O_5 ARC Layer	55-95 nm
Dielectric constant	11.9
Energy band gap	1.124 eV
Background doping P-type	1.513 × 10^{16} cm^{-3}
First front diffusion N-type	2.87 × 10^{20} cm^{-3}
Refractive index	3.42
Excitation mode	Transient
Temperature	25 °C
Other parameters	An internal model of PC1D
Primary light source	AM 1.5D spectrum
Bulk recombination time	10 μs
Constant light intensity	0.1 W/cm^2

3. Result and discussion

3.1 Crystalline and morphological properties

The Nb_2O_5 layer coated on the Si wafer with different thicknesses was analyzed in terms of crystalline phases by XRD measurements and morphological properties by FESEM. The XRD pattern of the Nb_2O_5 layer deposited on the silicon substrate shows that a pure phase with high crystallinity was formed. The XRD peaks of 001, 100, 101, and 002 are located at 22.57°, 28.52°, 36.71°, and 46.21° respectively, which confirms the deposition of Nb_2O_5.[34,35] The sharp XRD diffraction peaks at 66–70° are assigned to the typical Si phase,[36] validating the deposition of Nb_2O_5 on the silicon substrate as shown in Fig. 2. FESEM analysis has been used to measure the thickness of the Nb_2O_5 ARC layer on the textured Si wafer using the cross-sectional view, as shown in Figs. 3a-c. As seen in the FESEM images, Nb_2O_5 ARC thickness is decreased with the increase of spinning speed from 1000 to 3000 rpm. The cross-sectional view of the Nb_2O_5-coated on textured Si wafer ascertained the Nb_2O_5 thicknesses of 85, 75, and 65 nm at 1000, 2000, and 3000 rpm, respectively. Furthermore, the top view of the FESEM image further realizes the uniform deposition of the Nb_2O_5 layer on the Si wafer by the spin-coating technique, as shown in Fig. 3d. This experimentally measured thickness of Nb_2O_5 layers has been applied in the PC1D simulation for further characterization of photovoltaic properties.

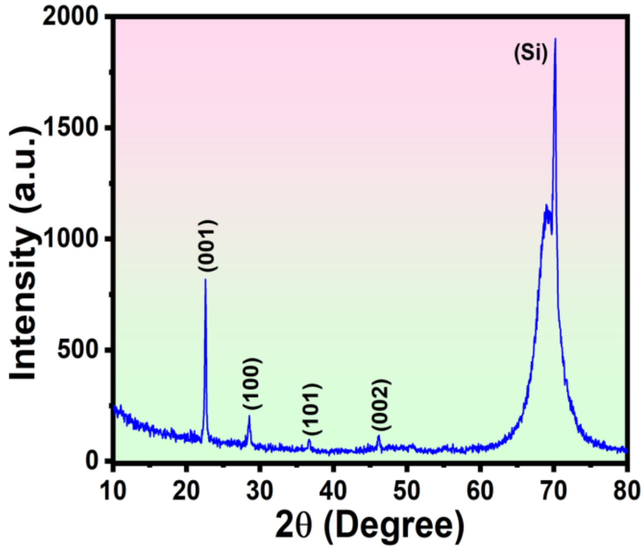

Fig. 2 XRD analysis of Nb_2O_5 deposited on a silicon substrate.

3.2 Optical properties

UV-DRS spectroscopy has been carried out to evaluate the reflectance at a different thickness of Nb_2O_5 ARC layers on the surface of the Si substrate. The reflectance analysis results presented the average reflectance of 26.3% for bare silicon, 12.19% for texture silicon, and 8.23%, 7.21%, and 9.14% for the thickness of Nb_2O_5 layer 85, 75, and 65 nm fabricated at 1000, 2000, 3000 rpm, respectively in the range of wavelength 400–1000 nm as shown in Fig. 4a. The thickness of the Nb_2O_5 ARC layer has been optimized by minimum reflectance,

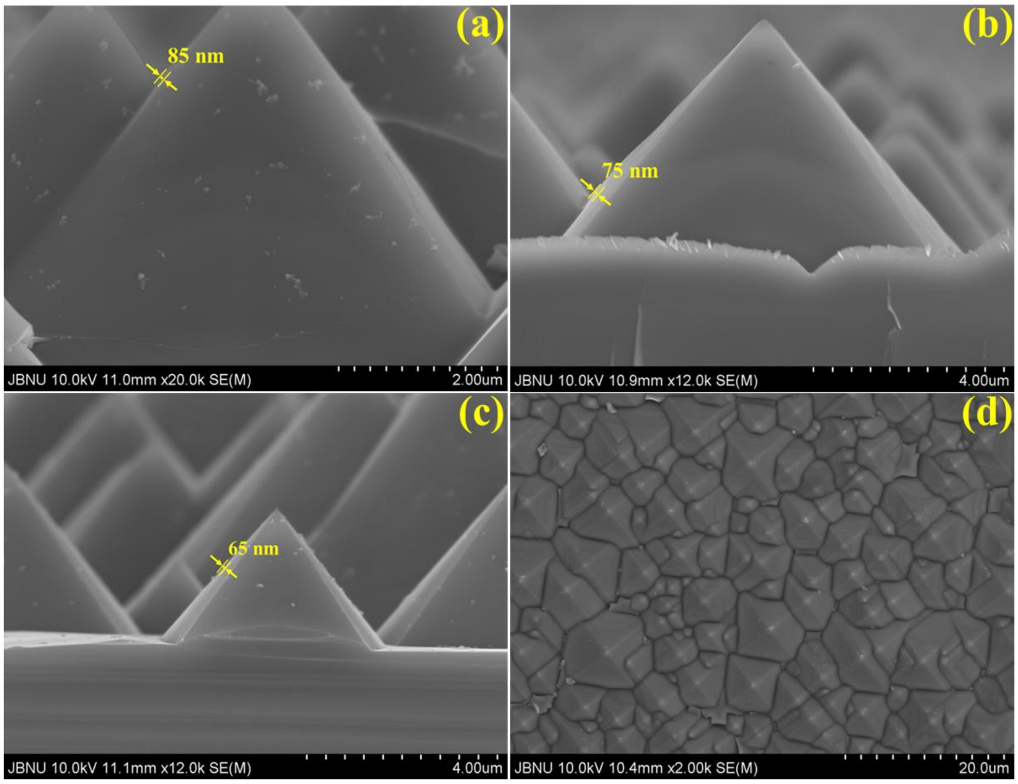

Fig. 3 FESEM images of a cross-sectional view of Nb_2O_5 deposited at spinning rate (a) 1000 rpm, (b) 2000 rpm, (c) 3000 rpm, and (d) FESEM image (top view) of Nb_2O_5 deposited on Si substrate.

which is exhibited at 75 nm deposited at a 2000 rpm spinning rate. The reflectance is lower at this thickness of the ARC layer because of an odd integer multiple of the quarter wavelength that corresponds to transmission inside the coating medium for a particular frequency and the thickness of ARC holds the situation of constructive interference more appropriately.[37] The simulation technique was also carried out for reflectance analysis, which exhibited 16.43%, 11.89%, 9.45%, 10.69, and 13.83% for 55, 65, 75, 85, and 95 nm, respectively, for the thickness of ARC layers as shown in Fig. 4b. The simulation results of reflectance are almost similar to the experimental measurement, which also validates the data. Reflectance values were used to compute refractive indices and extinction coefficients for all Nb_2O_5 ARC layers on the Si substrate.[38] The highest refractive index (n = 2.13) has been recorded for a thickness of 75 nm of the Nb_2O_5 layer as a comparison to other layers as shown in Fig. 5a, which is also favorable for efficient Si solar cells. Moreover, the extinction coefficient is also lowest for a thickness of 75 nm of Nb_2O_5 layer as a comparison to other layers as shown in Fig. 5b. The numerical values of refractive index and thicknesses of Nb_2O_5 layers deposited on the Si substrate at different spinning rates are listed in Table 2. Thus, Nb_2O_5 ARC material-based solar cell with low reflectance is highly advantageous for manufacturing efficient solar cells.

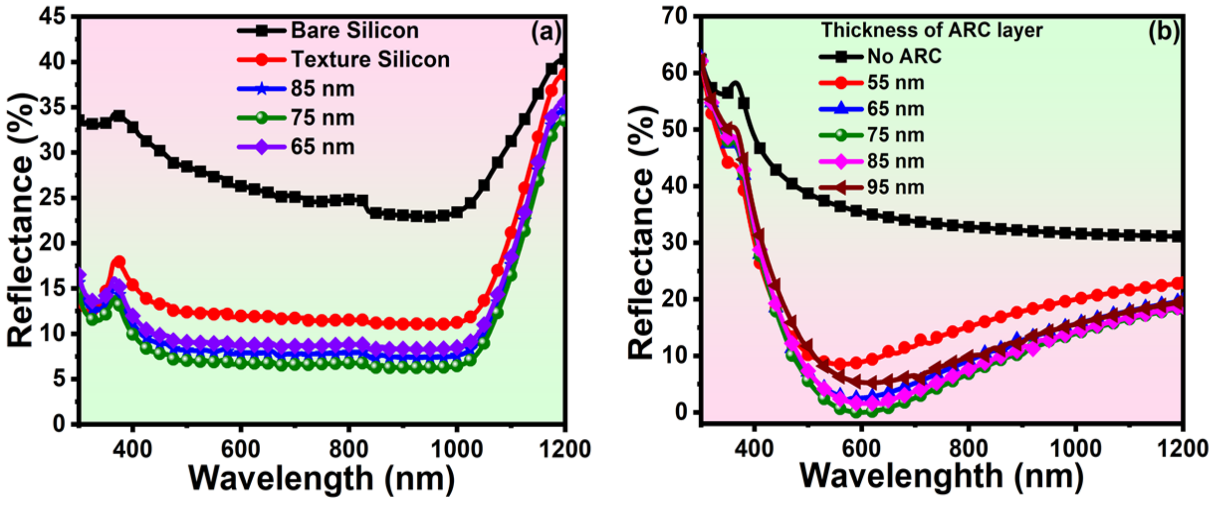

Fig. 4 Reflectance analysis by (a) experimental, (b) simulation of Nb_2O_5 deposited on Si substrate.

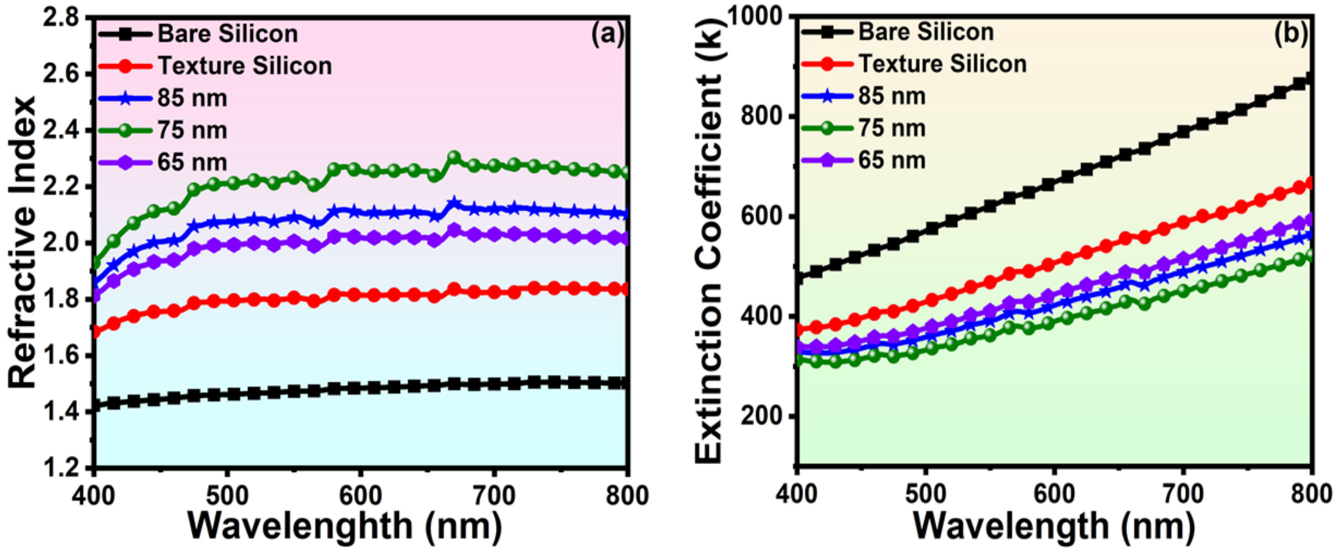

Fig. 5 Analysis of (a) refractive index, (b) extinction coefficient of Nb_2O_5 deposited on Si substrate.

Table 2. Photovoltaic parameters of Nb_2O_5 ARC layer-based c-Si solar cell.

Thickness of ARC Layer (nm)	Average Reflectance		Refractive Index		I_{sc} (A)	V_{oc} (V)	P_{max} (W)	FF (%)	Efficiency (%)
	Experimental	Simulation	Experimental	Simulation					
Bare/No ARC	26.40	36.17	1.47	--	2.28	0.642	1.22	69.80	12.27
55	--	16.43	--	2.70	3.03	0.649	1.653	83.70	16.53
65	9.14	11.89	1.97	2.33	3.21	0.651	1.751	83.73	17.51
75	7.21	9.45	2.18	2.00	3.28	0.651	1.792	83.76	17.92
85	8.39	10.69	2.05	1.75	3.24	0.651	1.769	83.74	17.69
95	--	13.83	--	1.57	3.14	0.650	1.713	83.74	17.13

The lifetime mapping images of the Nb_2O_5 ARC layer on a textured Si wafer with different thicknesses have been investigated to explain the surface bulk charge carrier lifetime.[39] In general, during the scanning of the Si wafer, the color changes define the minority carrier lifetimes. As a thickness of 75 nm, Nb_2O_5 ARC on Si wafer has been exhibited to have the lowest surface lifetime value as compared to other thicknesses, it suggests the optimized thickness of the Nb_2O_5 ARC layer on Si solar cells. With 75 nm thickness of ARC layer-based Si wafer, a decrease of the bulk lifetime from 0.9 µs to 11.2 μs is detected and manifests the lowering in the charge carriers, which might be beneficial for improving the optical properties as shown in Fig 6b. The lowest surface distribution of lifetime is 7.08 μs is optimum at 75 nm thickness of Nb_2O_5 ARC layer on Si solar cell in comparison with other samples, resulting in the low lifetime of bulk charge carriers on Si wafer as shown in Fig $6b_1$. The lifetime of charge carriers and their distribution might impact the optical behavior of AR surfaces.

To further define the photovoltaic parameters, it is important to have an accurate model which explains the uniform distribution of surface resistance or sheet resistance over the substrate.[40] The sheet resistance of Si substrate can affect the Isc, fill factor (FF), and hence the efficiency of a solar cell by contributing to the dispersed series resistance interconnecting gridlines and thus affects the total series resistance of a solar cell. Thus, the sheet resistance should be optimized to achieve excellent ohmic contact.[41] The sheet resistance increases with decreases in the thickness of Nb_2O_5 layers on the silicon substrate as shown in Fig. 7. The maximum sheet resistance ~222.42 Ω/sq is recorded at a thickness of 75 nm (deposited at 2000 rpm), which is also favorable for efficient solar cells.

3.3 Photovoltaic properties

The efficiency (η) of the solar cells is calculated by using the equation (1)[32];

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{oc}*I_{sc}*FF}{P_{in}} \quad (1)$$

where V_{oc} is the open-circuit voltage, I_{sc} is the short-circuit current, and FF is the fill factor. The FF determines the maximum power from the solar cells, and explains the ratio of the real output from the solar cell ($V_{mp} \times I_{mp}$) to the product of $V_{oc} \times I_{sc}$, as expressed by below equation (2)[32];

$$FF = \frac{V_{mp}*I_{mp}}{V_{oc}*I_{sc}} \quad (2)$$

where V_{mp} is the value of the voltage for the maximum power from a solar cell, and I_{mp} is the value of the current for the maximum power from a solar cell. The I-V curve is the crucial

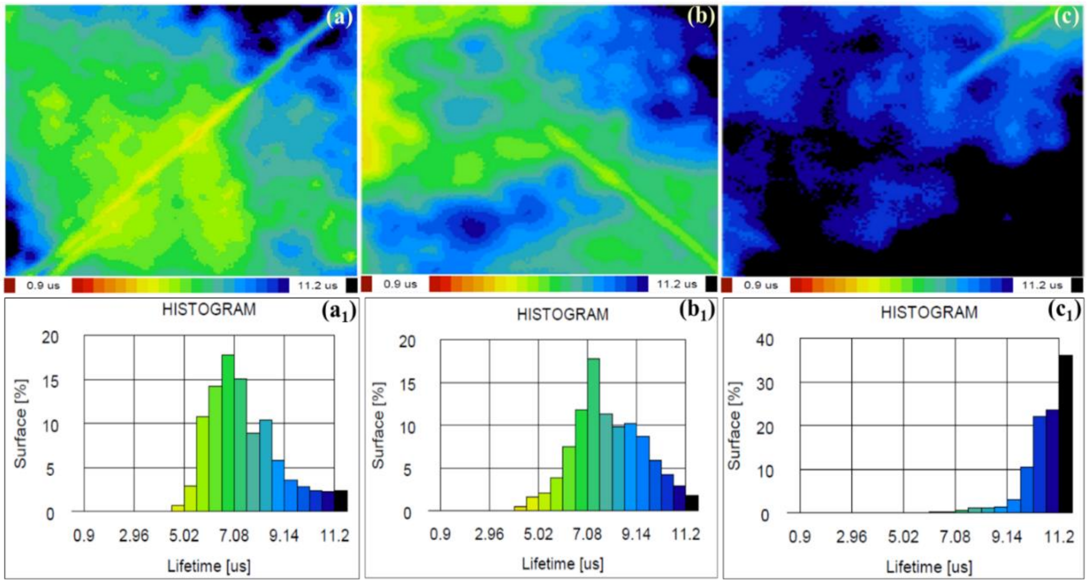

Fig. 6 Carrier Lifetime distribution and histogram analysis of Nb_2O_5 deposited at spinning rate (a, a_1) 1000 rpm (b, b_1) 2000 rpm (c, c_1) 3000 rpm on Si substrate.

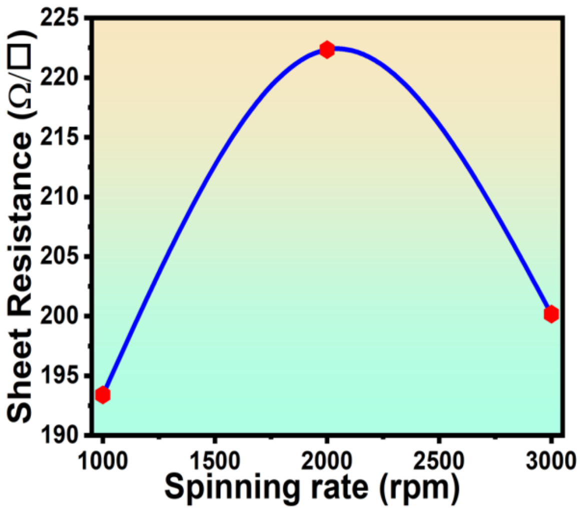

Fig. 7 Analysis of sheet resistance with ARC layer deposited at different spinning rates.

property to manufacture efficient solar cells. The highest I_{sc} = 3.28 A, V_{oc} = 0.651 V has been observed for ARC-based solar cells as shown in Fig. 8a. The highest photocurrent of solar cells has been achieved due to an increase in the effectiveness of the absorption of a photon. The highest power 1.92 W and a fill factor of 83.76% have been recorded for ARC-based silicon solar cells during the simulation and other electrical properties have been summarized in Table 2. The ratio of photogenerated carriers per incident photon as a function of wavelength is known as the external quantum efficiency (EQE).[42,43] The performance of ARC layer-based solar cells in terms of EQE was studied by changing the different thicknesses of the ARC layer from 55 nm to 95 nm. It has been found that EQE at 75 nm thickness ARC-based silicon solar cells exhibited more than 95% in the range of wavelength 300–1200 nm among all thicknesses as shown in Fig. 8b.

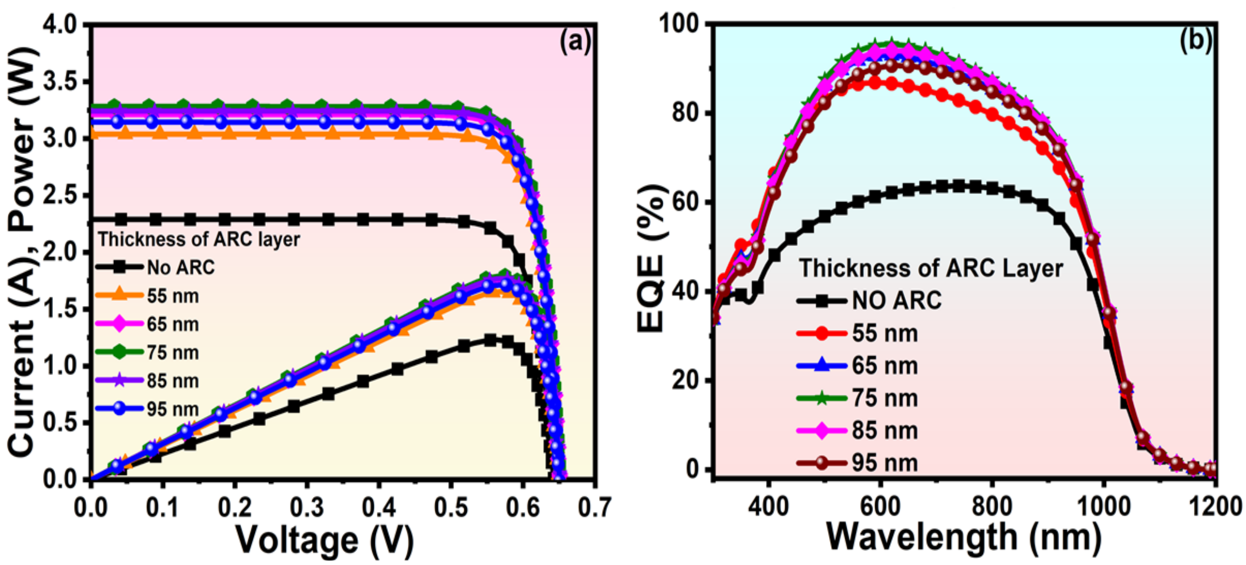

Fig. 8 Analysis of (a) I, P-V curve, (b) quantum efficiency of Nb_2O_5 ARC layer-based c-Si solar cell.

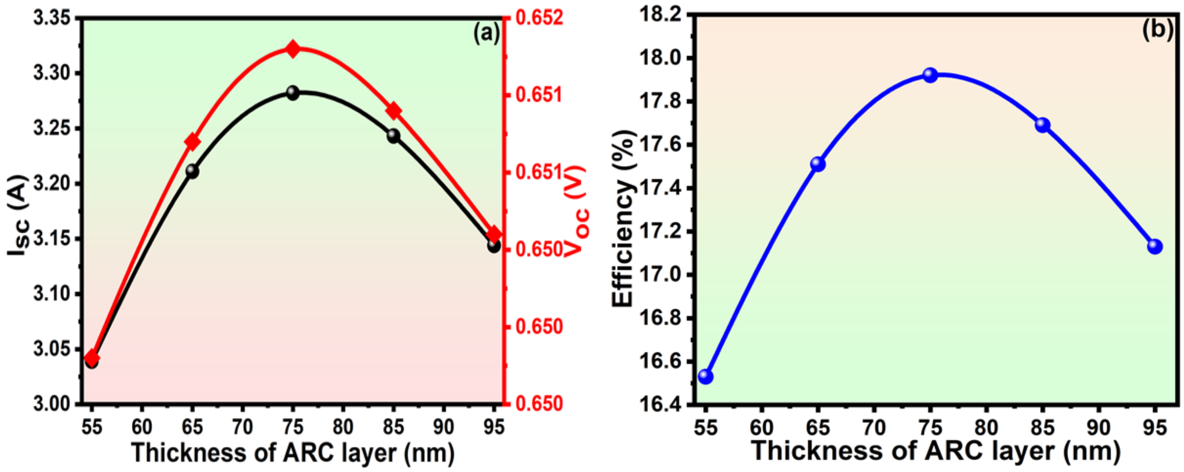

Fig. 9 Analysis of (a) I_{sc} & V_{oc} curve, (b) efficiency of Nb_2O_5 ARC layer-based c-Si solar cell.

Table 3. Comparative study of PV parameters of Nb_2O_5 based solar cell.

Types of Solar cell	I_{sc} (A)	V_{oc} (V)	FF (%)	Efficiency (%)	References
Ga: $ZnO/Nb_2O_5/Si$	0.60	0.64	72.02	9.32	[44]
Nb_2O_5/Si	5.06	2.90	65.05	15.23	[45]
Nb_2O_5/TiO_2/DSSC	0.10	0.62	65.00	5.23	[46]
Nb_2O_5/Si	3.28	0.65	83.76	17.92	This work

As the thickness of the ARC layer increases, the I_{sc} and V_{oc} of solar cell increase up to 75 nm and after that, it starts to decrease on further increasing as shown in Fig. 9a. The decrease on further increasing as shown in Fig. 9a. The highest I_{sc} = 3.28 A and V_{oc} = 0.651 V have been observed at ARC thickness 75 nm. This is due to the thickness of ARC holding the condition of constructive interference more properly at 75 nm.[47] As the path difference between the light rays reflected from the top and bottom surface of the ARC is less than $\lambda/4$, it does not support injecting the light into the solar cell properly at this structure.[48] After more than 75 nm thickness of ARC, the reflectivity decreases linearly because ARC holds the condition of destructive interference more properly.[49,50] At 75 nm thickness of the ARC layer, the condition of destructive interference achieves perfectly and presents the minimum reflectivity. The highest efficiency (η = 17.92%) has been achieved at 75 nm thickness of the ARC layer as shown in (Fig. 9b). Furthermore, the electrical parameters of reported ARC material-based solar cells have been summarized in Table 2. By comparing these electrical parameters, Nb_2O_5 ARC-based solar cells exhibited better results as a comparison to others and might be suitable for manufacturing proposed solar cells. The comparative study of the proposed solar cell also confirms the simulated parameters of the Nb_2O_5 ARC-based solar cell by the PC1D simulation software as shown in (Table 3).

Photogeneration of the electron is the gain of energy and moves from the valance band to the conduction band. The generation of an electron-hole pair can be calculated at any location within the solar cell, at any wavelength of light, or for the entire standard solar spectrum. The generation rate provides the number of electrons generated at each point in the device due to the absorption of photons.[51] The solar cell's photogeneration rates are crucial in estimating high charge generation and charge collecting.[52] The photogeneration rate has been started from 0/sec and gradually increases with an increase in the distance from the front of the solar cell. The highest photogeneration rate is 2.23 × 10^{19}/s for Nb_2O_5 ARC-based solar cells as the comparison to other layers as shown in Fig. 10. As can be seen in Fig. 10, the deposition of Nb_2O_5 ARC is very crucial to facilitate the photogeneration rate. The generation rate is the greatest at the surface of the material, where most of the light is absorbed.[51] The maximum photogeneration rate is recorded when the thickness of Nb_2O_5 ARC is 75 nm. Importantly, the high photogeneration rate

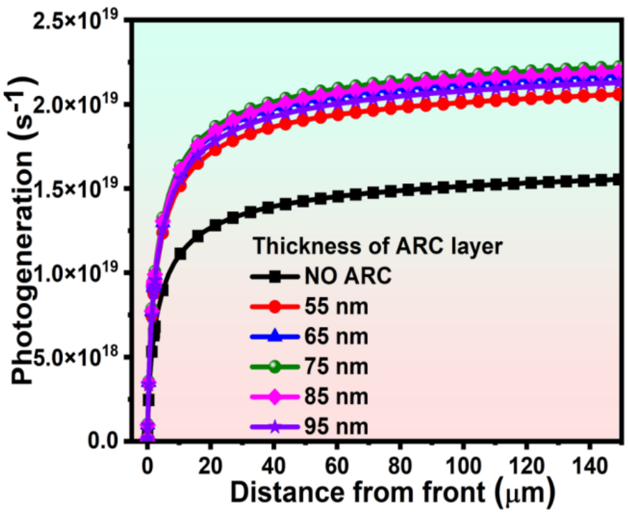

Fig. 10 Analysis of photogeneration analysis of Nb_2O_5 ARC layer-based c-Si solar cell.

matches the high charge generation rate, as a result of the high photocurrent and high performance of the Nb_2O_5 ARC layer-based solar cell.

4. Conclusion

A low-cost sol-gel derived spin coating method was used to optimize the thickness of the Nb_2O_5 ARC layer on a c-Si solar cell and successfully characterized the optical, structural, crystalline, charge carrier generation, and photovoltaic properties. In support, a simulation approach was successfully performed to explore and validated the optoelectrical and photovoltaic properties of the Nb_2O_5 ARC layer-based c-Si solar cell. In a simulation study, the different thicknesses of the Nb_2O_5 ARC layer were selected as input parameters to explore the photovoltaic characteristics of c-Si solar cells. The optical characterization revealed that the lowest average reflectance of ~7.21% was achieved when Nb_2O_5 ARC thickness was 75 nm. The simulated results showed that the highest PCE of 17.92% was recorded at 75 nm thickness of the Nb_2O_5 ARC layer. From obtained results, the optimized thickness (75 nm) of the Nb_2O_5 ARC layer exhibited the highest performance, photocurrent, and external quantum efficiency (EQE) of 95%. This simulation on the optimization of thicknesses of the ARC layer for Si solar cells would provide the utilization of low-cost Nb_2O_5 ARC layer-based for the development of high-performance c-Si solar cells.

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Conflict of interest

There are no conflicts to declare.

Supporting information

Not applicable.

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