

ENHANCEMENT IN SOLAR CELL EFFICIENCY BY USING $\text{Al}_2\text{O}_3/\text{TiO}_2$ AS A PASSIVATION LAYER IN PERC TYPE SOLAR CELL SIMULATION USING TCAD

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Abstract

In this study, we utilized high-k materials and their stacks for surface passivation in high-efficiency crystalline silicon passivated emitter rear contact (PERC) solar cells. The $\text{Al}_2\text{O}_3/\text{TiO}_2$ stack was employed as a potential passivation layer materials to minimize the recombination losses. In this configuration, Al_2O_3 functions as a passivation layer, while TiO_2 serves as a capping layer. We have also optimized the half pyramid length and demonstrated its impact on the efficiency of the solar cell. The efficiency of the PERC solar cells of different half pyramid length were compared with the Al-BSF solar cell. Additionally, we investigated and optimized the effects of varying the thickness of the Al_2O_3 layer in the stack passivation structure was also investigated and optimized. Al_2O_3 passivation layer of three different thickness 6, 8, and 10 nm were used and its effect on efficiency were analyzed. The Fill factors and Open circuit voltage for different half-length of pyramid were also measured. An efficiency improvement of approximately 1.2% was observed in the PERC solar cell structure with the $\text{Al}_2\text{O}_3/\text{TiO}_2$ stack layer.

Keywords: Efficiency Improvement; Fill Factor; PERC Solar Cell; Surface Passivation

Introduction

The global demand for energy is increasing at an unprecedented rate, with projections indicating that it will double by 2050. This rapid surge in energy consumption has created an urgent need to explore and expand energy resources to meet future requirements (Wagner *et al.*, 2024; Ziar, 2024). Traditionally, the energy landscape has been dominated by non-renewable resources such as coal, oil, and natural gas, which currently account for approximately 80% of the world's energy supply.

However, these fossil fuels are being depleted at an alarming rate and present significant environmental challenges, including greenhouse gas emissions and climate change (Overland *et al.*, 2022). Consequently, it has become imperative to explore sustainable and eco-friendly alternatives to ensure a reliable energy supply for future generations.

Among the various renewable energy sources available, photovoltaic (PV) technology stands out

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as one of the most promising and rapidly growing solutions. Photovoltaic systems harness solar energy and convert it into electricity using solar cells. Currently, silicon-based solar cells dominate the PV market, accounting for nearly 90% of the global market share. Despite their widespread adoption, further cost reductions are essential to facilitate the mainstream integration of solar power into global electricity generation. One effective approach to achieve cost reductions is by minimizing the thickness of silicon wafers used in solar cells (Sun *et al.*, 2022). However, this approach introduces challenges related to the recombination of charge carriers, which significantly affects the efficiency of the cells.

Charge carrier recombination remains a primary loss mechanism in silicon solar cells (Richter *et al.*, 2021). Extensive research has been conducted to address this issue and enhance the efficiency of solar cells. A significant portion of recombination losses occurs at the silicon surface. As the thickness of the substrate continues to decrease to reduce production costs, surface passivation has become increasingly critical. Surface passivation involves applying specific materials to the silicon surface to reduce the density of surface trap states, thereby minimizing recombination losses (Muduli and Kale, 2023).

High-k dielectric materials have emerged as effective solutions for surface passivation, as they help mitigate charge carrier recombination losses by reducing surface trap densities (Grandhi *et al.*, 2024). Traditionally, silicon dioxide (SiO₂) and silicon nitride (SiN_x) have been used as passivation materials. While SiN_x provides passivation benefits, it also presents challenges due to its positive charge, which can reduce the density of majority carriers at the surface (Chen, 2025). This reduction in carrier density can lead to parasitic shunting in passivated emitter rear contact (PERC) solar cells, particularly those based on p-type silicon substrates.

To overcome these limitations, aluminum oxide (Al₂O₃) has been proposed as a superior alternative to SiN_x for surface passivation (Bansal *et al.*, 2019). Al₂O₃ possesses a high concentration of negative charges, making it highly effective in passivating the silicon surface and reducing recombination losses. In addition to its excellent passivation properties, Al₂O₃ offers long-term stability and compatibility with existing silicon solar cell manufacturing processes. However, Al₂O₃ films exhibit a relatively low refractive index, which limits their effectiveness as anti-reflection coatings (ARCs). Anti-reflection coatings are crucial for enhancing the light absorption efficiency of solar cells by minimizing reflection losses at the cell surface (Alkallas *et al.*, 2024).

To address this challenge, researchers have proposed the use of Al₂O₃/TiO₂ stack structures. These stacks combine the superior passivation properties of Al₂O₃ with the excellent anti-reflection capabilities of titanium dioxide (TiO₂). TiO₂, known for its high refractive index, serves as a capping layer, effectively reducing reflection losses and enhancing light absorption. The combination of Al₂O₃ and TiO₂ not only improves the optical performance of the solar cells but also provides additional benefits in terms of surface passivation (Zhang *et al.*, 2021).

The use of Al₂O₃/TiO₂ stack structures further reduces the surface recombination velocity, a critical parameter that determines the efficiency of solar cells. This improvement is attributed to the hydrogenation of Si/Al₂O₃ interface states. During the passivation process, hydrogen atoms diffuse into the silicon/Al₂O₃ interface, effectively passivating the defect states and reducing the density of interface traps. As a result, the surface recombination velocity decreases, leading to higher carrier lifetimes and improved overall cell efficiency (Colonna *et al.*, 2020).

Moreover, Al₂O₃/TiO₂ stack structures provide additional advantages in terms of mechanical stability and durability. The robust nature of these stacks ensures long-term performance, even under challenging environmental conditions. This stability is crucial for the widespread deployment of solar energy systems, particularly in regions with extreme weather. The integration of Al₂O₃/TiO₂ stack structures into silicon solar cells represents a significant advancement in photovoltaic technology (Szindler *et al.*, 2022). By combining superior passivation with effective anti-reflection properties, these stack structures pave the way for high-efficiency, cost-effective solar cells. As research and development efforts continue to refine this technology, the widespread adoption of Al₂O₃/TiO₂-based solar cells is expected to accelerate, further driving down the cost of solar energy and promoting its integration into mainstream electricity generation.

In this paper, we use Silvaco TCAD to simulate the PERC solar cell structure on a p-type Si substrate and use Al₂O₃/TiO₂ stacks for back surface passivation. A layer of TiO₂ was used on the top for its anti-reflection properties. Our focus is on stacks where the Al₂O₃ layer is thin (in the order of 0.010 μm or less) and has negligible effect on the optical properties of the stack. We investigate the changes in efficiency resulting from variation in length of the pyramids on top of the cell and the thickness of Al₂O₃.

Simulation Strategy and Results for Al-BSF and PERC type Solar Cell

Silvaco TCAD tool has been utilized for the design and characterization of Al BSF and PERC solar cell structures (Kashyap *et al.*, 2022; Salem *et al.*, 2022; Boukortt *et al.*, 2024). Silvaco simulation tools, including ATHENA, ATLAS, DEVEDIT and TONYPLOT were employed for the design, characterization and graphical representation of the structures and their characteristics. Athena primarily creates the structure and determines the fundamental etching and deposition processes. Various virtual wafer fabrication tools that are used in ATHENA includes SSUPREM4, ELITE and OPTOLITH. ATLAS is a simulation tool that simulates devices physically. It provides two-dimensional and three-dimensional semiconductor device simulation. For specified biased conditions, ATLAS calculates the electrical characteristics of devices which it has taken as input from ATHENA and DEVEDIT. DEVEDIT is used to define structure of device and generate a new mesh on an existing structure. It can also be used to modify an existing device structure. For the solar cell surface passivation, ATLAS deals with the various models like Shockley-Read-Hall recombination, Auger recombination, Radiative recombination, and surface recombination (Bansal *et al.*, 2024). Apart from these recombination models, a number of partial-differential equations are used for describing the distribution of carrier current such as Poisson's equation, Continuity equation and Transport equations (Ayobi, 2022). Newton mathematical technique was used for the calculation and maximum iteration limit was set to 50. Luminous optoelectronic simulator was used for simulations in this research work. Luminous calculates the optical intensity profiles of the semiconductor and converts it into the photo-generation rates (Roy *et al.*, 2021). DEVEDIT can create both 2D and 3D device structures. DEVEDIT provides semi-automatic re-meshing of pre-existing structures. It reduces the simulation time by re-meshing the structures created by process simulation in ATHENA before they are used for de-vice simulation in ATLAS. Finally, TONYPLOT is used to visualize the TCAD structures (1D, 2D, and 3D) generated by silvaco TCAD simulators. It processes the data files and plots the generated results from the log files and structure files of the device. During the simulation various physical models used in the present investigation for solar cell modeling in ATLAS can be divided into two categories: (i) Mobility, and (ii) Recombination.

Mobility, as a function of doping concentration, is specified by using the CONMOB parameter in the mobility statement. The default values for the mobility of electrons and holes for specific doping concentrations are defined in ATLAS.

Whereas the recombination model calculates the carrier lifetimes when semiconductors are disturbed from their equilibrium condition, Shockley-Read-Hall (SRH) model is the most commonly used framework for modeling the surface passivation of solar cells (Nakamura *et al.*, 2021). The effect of recombination is modeled in the presence of traps (or defects) within the forbidden gap of the semiconductor. SRH recombination in ATLAS is modeled as follows:

$$R_{SRH} = \frac{pn - n_{ie}^2}{TAUP0 \left[n + n_{ie} \exp\left(\frac{E_{TRAP}}{kT_L}\right) \right] + TAUN0 \left[p + n_{ie} \exp\left(\frac{-E_{TRAP}}{kT_L}\right) \right]} \quad (1)$$

where, E_{TRAP} is the difference in trap energy level and intrinsic fermi level. T_L is the Temperature in degree Kelvin, TAUP0 and TAUN0 are the user defined holes and electrons lifetimes parameters in MATERIAL statement.

This model is activated in simulation by using the SRH parameter in MODEL statement in simulation. The Auger recombination is important in case of high carrier densities (Sravani *et al.*, 2021). It is modelled in ATLAS as

$$R_{Auger} = AUGN(pn^2 - nn_{ie}^2) + AUGP(np^2 - pn_{ie}^2) \quad (2)$$

where, AUGN and AUGP are user defined parameters in MATERIAL statement. This model is activated by using the AUGER parameter in model statement.

For the simulation of a solar cell, a P-type silicon wafer with a thickness of 275 μm , an orientation of $\langle 100 \rangle$, and a resistivity of 1 $\Omega\text{-cm}$ has been utilized. The front side was textured using geometric silicon etching. Pyramidal etching was carried out on the silicon surface to enhance light trapping, and consequently, the efficiency of the solar cell, as reflection control alone has limited potential for absorption enhancement.

The emitter diffusion was conducted with a sheet resistance of 90 $\Omega\text{-cm}$ to form a n^+ region through phosphorus doping, utilizing an implant dose of 5×10^{17} for 30 min at 900°C. An anti-reflection coating of SiN_x of thickness 0.070 μm was applied to the top of the cells. Aluminum metal contacts were added to create the cathode and anode. After modeling and completing the basic solar cell

for different lengths of the pyramid (Length_half_pyramid taken = 2, 3, 4, 5, 6, 7 microns) as shown in Figure 1, we initiated the process of depositing a passivation layer of dielectric materials to investigate the improvements in efficiency.

We compare two control models. The first is an aluminum back surface field (Al-BSF) solar cell which is an industrially produced solar cell which is readily available today. The second structure is a passivated emitter rear cell (PERC) solar cell featuring a back surface passivated with a 0.010 μm Al₂O₃ film. Additionally, a 0.070 μm SiN_x film, used as an antireflection coating, was deposited on top of the cell.

The third simulation involved our proposed model, which utilized a stack of Al₂O₃ and TiO₂ was used on the back surface along with a TiO₂ anti-reflection coating (ARC) on the front surface.

The thickness of Al₂O₃ for the initial run was selected to be 0.010 μm , while the thickness of TiO₂ was set at 0.050 μm (For AR index – 2.43). This choice was made to remain close to the theoretically optimized thickness, as indicated by:

$$d_{ARC} = \frac{\lambda}{4n_{ARC}} \quad (3)$$

and

$$n_{ARC} = \sqrt{n_{Si} n_{ambient}} \quad (4)$$

with d the ARC thickness and n the refractive indices of the materials. TiO₂ has n (ambient) = 2.43 according to which for n (Si) = 3.8 we get n (ARC) = 3.04. For a system optimized for the peak intensity of sun light (0.633 μm) the resulting ARC thickness is 0.052 μm . Hence the 0.050 μm TiO₂ layer was chosen.

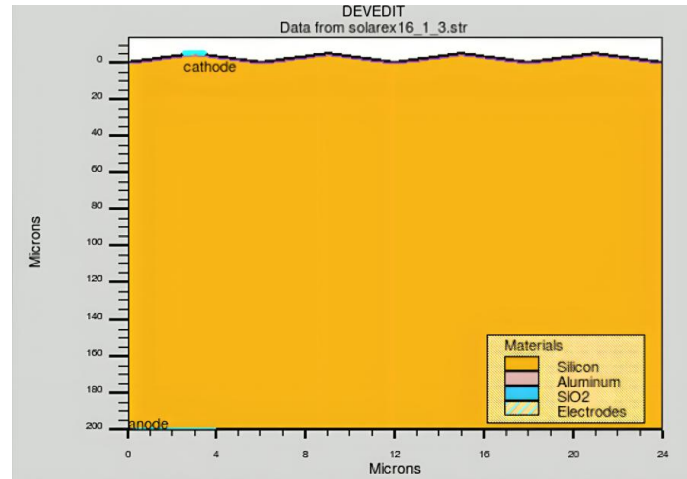


Figure 1. Different Length_half_pyramid structures

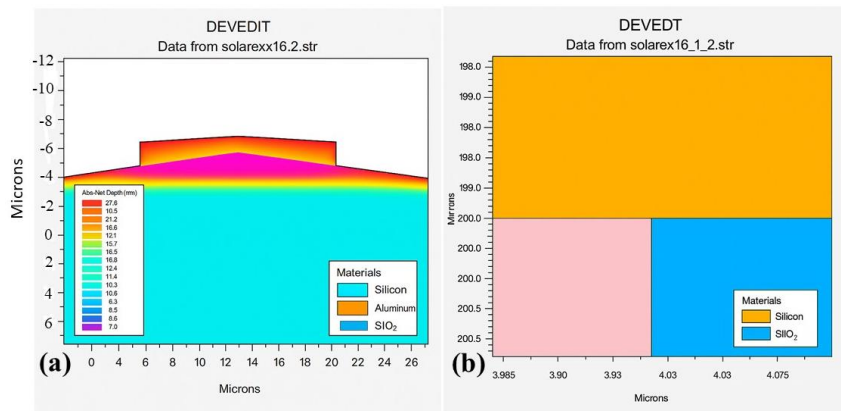


Figure 2. Al-BSF solar cell structure with (a) Cathode contact (Doping Gradient/Contour) (b) Anode Contact (SiO₂ layer on Back Surface)

Aluminum Back Surface Field (Al-BSF) Structure

Case 1: SiO₂ (Back Surface | Thickness = 0.70 μ m) - SiN_x (Anti Reflection Coating | Thickness = 0.070 μ m)

The Al-BSF structure was designed using SiO₂ as a passivation layer and SiN_x as an antireflection coating, as shown in Figure 2. The thickness of the SiO₂ and SiN_x layers were of 0.7 μ m and 0.070 μ m, respectively. The top view of the Al-BSF and PERC solar cell structures was modeled in silvaco TCAD. On the top of the designed Al-BSF and PERC structures, no passivation layer has been deposited in order to keep the design simple for comparison purpose as shown in Figure 2. Full rear metal coating was applied to the Al-BSF structure.

Passivated Emitter Rear Contact (PERC) Structure

Al₂O₃ (Back Surface Passivation | Thickness = 0.010 μ m) - SiN_x (Anti Reflection Coating | Thickness = 0.070 μ m)

The first PERC structure was constructed by depositing the 0.010 μ m thickness of Al₂O₃ and the 0.070 μ m thickness of SiN_x on the rear side of the solar cell as shown in Figure 3.

Al₂O₃ (Back Surface Passivation | Thickness = 0.010 μ m) – TiO₂ (Anti Reflection Coating | Thickness = 0.070 μ m)

The second PERC structure was constructed by depositing variable thickness of Al₂O₃ (0.006, 0.008, 0.0010 μ m) and fixed thickness of TiO₂ (0.050 μ m) on the rear side of the solar cell. In this configuration, the TiO₂ layer serves as an anti-reflection coating. The permittivity values for the Al₂O₃ and TiO₂ layers have been taken as 9 and 85. The contact electrode has been shown in Figure 2. When a-SiN_x layer is deposited as a capping layer on Al₂O₃, it increases the extinction coefficient, which is not desirable for solar cell applications (Canar *et al.*, 2023). Therefore, a TiO₂ capping is preferred over a-SiN_x because of its moderate extinction co-efficient and high refractive index. Another advantage of TiO₂ capping is that

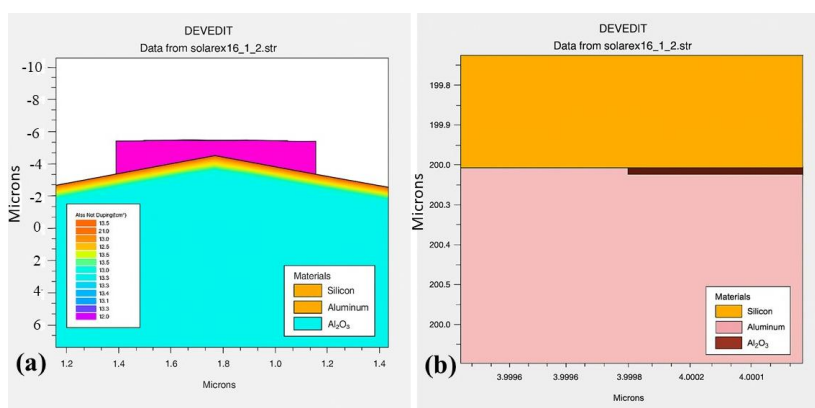


Figure 3. PERC solar cell structure with (a) Cathode contact (Doping Gradient/Contour) (b) Anode Contact (Al₂O₃ layer on Back Surface)

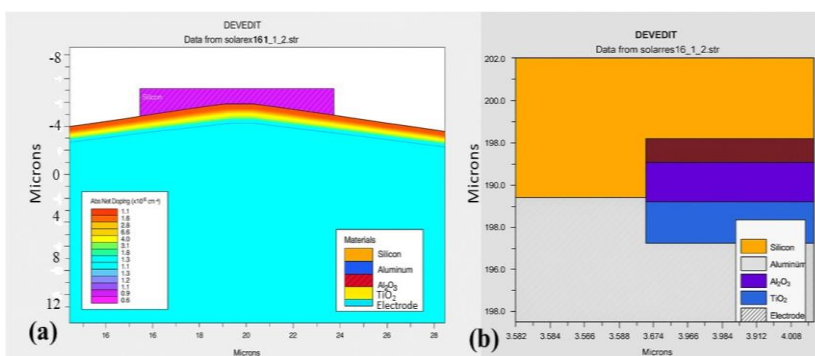


Figure 4. (a) Cathode contact (Doping Gradient/Contour). (b) Anode Junction (Al₂O₃/TiO₂ BS stack)

it can be deposited along with Al₂O₃ within the same chamber (Figure 4). The refractive index of TiO₂ can be graded, and the ALD process which can further reduce its optical reflectance (Jha *et al.*, 2020). With the TiO₂ capping layer, the accumulation capacitance was found to increase, resulting in reliable CV characteristics. As the thickness of the Al₂O₃ layer increases, the significance of TiO₂ for passivation diminishes. It has been observed that the negative charge increases with TiO₂ capping, which enhances the field effect passivation and reduces the D_{it} level leading to improved chemical passivation (Suh and Kang, 2017). The decrease in D_{it} level is attributed to the release of atomic hydrogen following the deposition of the TiO₂ layer which can be further enhanced through annealing.

Results and Discussions

Electrical Characteristics

The open circuit output voltage (V_{oc}) and short circuit output current density (J_{sc}) were obtained for all the three samples (i) Al-BSF, (ii) Al₂O₃-SiN_x, and (iii) Al₂O₃-TiO₂.

Figure 5 depicts the variation of open circuit output voltage (V_{oc}) with respect to length of pyramid due to its impact on optical, electrical, and recombination properties of the solar cell. the open-circuit voltage varies with pyramid length due to competing effects of light absorption and surface recombination. As pyramid length increases, light trapping improves, enhancing carrier generation and initially raising V_{oc} (Wang *et al.*, 2021a). However, larger pyramids also increase surface area, leading to higher surface recombination, which reduces V_{oc} if not properly passivated (Wang *et al.*, 2021b). There exists an optimal pyramid length (typically 2–8 μm) that balances enhanced absorption with minimal recombination losses. Beyond this, V_{oc} declines despite better light absorption. Proper surface passivation is essential for mitigating these recombination effects and maintaining a high V_{oc} (Wu *et al.*, 2023). In PERC solar cells that utilize Al₂O₃ as a passivation layer, the open-circuit voltage (V_{oc}) and short-circuit current density (J_{sc}) exhibit a logarithmic relationship described by $V_{oc} \propto \ln(J_{sc})$, assuming a constant dark saturation current density (J_0). An increase in J_{sc} , resulting from enhanced light

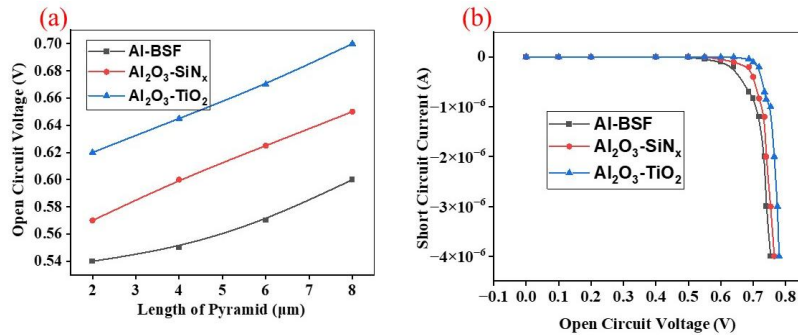


Figure 5. Output characteristics of PERC type Solar cell (a) V_{oc} vs length of pyramid, and (b) Short circuit cathode current vs V_{oc}

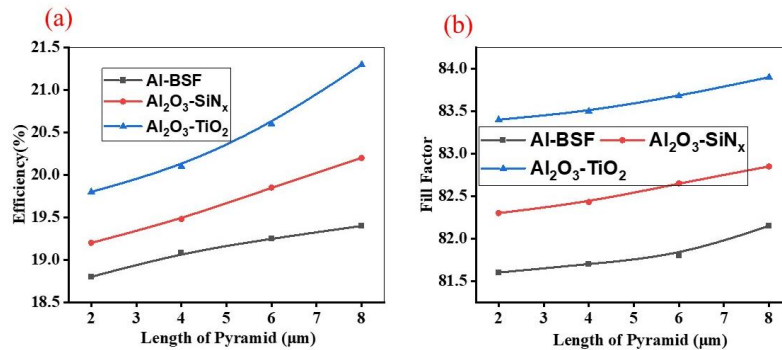


Figure 6. (a) Efficiency and (b) Fill factor variation with respect to length of pyramid

absorption, typically leads to a higher V_{oc} , although the benefits may diminish at higher levels. The passivated rear surface in PERC cells reduces recombination, which helps maintain a low J_0 and enhances V_{oc} . However, excessive recombination can negate this advantage, limiting V_{oc} even in the presence of increased J_{sc} . Therefore, optimizing passivation and minimizing recombination are crucial to ensure that improvements in J_{sc} effectively translate into higher V_{oc} .

In Al-BSF and PERC solar cells, efficiency varies with pyramid length due to differences in light trapping and recombination behaviour as shown in Figure 6.

For Al-BSF cells, short pyramids ($\sim 1\text{--}2\text{ }\mu\text{m}$) lead to inadequate light absorption, while medium pyramids ($\sim 5\text{--}10\text{ }\mu\text{m}$) optimize efficiency by enhancing J_{sc} . For PERC cells, which have rear passivation layer of Al_2O_3 , both light trapping and V_{oc} improve significantly with increased pyramid length. Efficiency reaches its peak at $8\text{ }\mu\text{m}$, as PERC cells reduce recombination losses more effectively than Al-BSF cells (Choi *et al.*, 2025). However, excessive pyramid length still increases front-surface recombination, resulting in a slight decrease in efficiency.

Overall, PERC benefits more from pyramid texturing than Al-BSF due to superior passivation. Optimizing pyramid length is essential to balancing light absorption and recombination losses to achieve maximum efficiency. $\text{Al}_2\text{O}_3/\text{TiO}_2$ stacks offer symmetrical passivation, delivering comparable performance on both n-type and p-type Si substrates. Additionally, these stacks enhance the electrical conductivity of the passivation layer without significantly compromising its performance. When TiO_2 is used as an anti-reflection coating (ARC), it further enhances light absorption by reducing surface reflections, thereby positively influencing the efficiency of both Al-BSF and PERC solar cells.

With TiO_2 anti-reflection coating (ARC), solar cells exhibit improved light absorption and higher J_{sc} , but its direct effect on fill factor (FF) is minimal. In Al-BSF cells, FF shows a slight improvement with pyramid lengths of $5\text{--}10\text{ }\mu\text{m}$ due to enhanced absorption, but it declines beyond this range as surface recombination and series resistance (R_s) increase. In PERC cells, TiO_2 enhances absorption while rear passivation minimizes recombination, keeping FF higher and more stable, peaking at $5\text{--}15\text{ }\mu\text{m}$. PERC benefits more from TiO_2 than Al-BSF because of reduced recombination losses, ensuring better FF retention at longer pyramid lengths. Optimal pyramid design is essential for maximizing efficiency.

Conclusions

This study investigates the enhancement of solar cell efficiency by employing an $\text{Al}_2\text{O}_3/\text{TiO}_2$ stack as a passivation layer in Passivated Emitter Rear Cell (PERC) solar cells. The Al_2O_3 layer functions as a passivation layer, while the TiO_2 layer serves as a capping layer to reduce recombination losses. Various half pyramid lengths and Al_2O_3 thicknesses (0.006 , 0.008 , and $0.010\text{ }\mu\text{m}$) were optimized to analyse their effects on solar cell efficiency. The results indicate a significant efficiency boost of approximately 1.2% with the $\text{Al}_2\text{O}_3/\text{TiO}_2$ stack compared to Al-BSF solar cells. The TiO_2 with an AR index of 2.43 serves as an excellent optical confiner. Additionally, the passivation stack enhances the internal light reflection at the rear side of the PERC solar cell resulting in a substantial improvement of the quantum efficiency. This research emphasizes the critical role of surface passivation in minimizing charge carrier recombination, which is essential for enhancing the performance of silicon solar cells. Simulations were conducted using Silvaco TCAD tools to model and characterize the solar cell structures.

Data Availability Statement

The data used in this work included in this manuscript.

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Disclosure

The author does not have any conflict of interest to disclose.

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