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Simulation-Based Optimisation of Anti-reflective Coating Materials for Si(n+)/Si(p) Heterojunction Silicon Solar Cells

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ABSTRACT: This study investigates electrical and optical losses in silicon heterojunction (SHJ) solar cells. It evaluates single-layer anti-reflective coatings (ARCs), including silicon dioxide (SiO_2), magnesium fluoride (MgF_2), magnesium oxide (MgO), titanium nitride (TiN) and aluminium oxide (Al_2O_3) to enhance light absorption and carrier generation. A one-dimensional PC1D simulation is used to model the device's electrical and optical behaviour and to predict key parameters, including short-circuit current density (JSC), open-circuit voltage (VOC), fill factor (FF) and power conversion efficiency (PCE). It is also used to evaluate external quantum efficiency (EQE) and reflectance while optimising ARC layer properties. Results reveal that MgO delivers the best performance, achieving a peak VOC of 656 mV, JSC of 15.39 mA/cm², EQE of 93.1% at 630 nm and a minimum reflectance of 6.80%. Al_2O_3 and TiN follow closely, with EQE values of 92.98% and 92.83%, respectively, and reflectance minima of 6.91% and 7.05%, respectively. Meanwhile, SiO_2 and MgF_2 exhibit lower efficiencies, with peak EQE values of 83.73% and 86.27%, respectively. Overall, MgO, Al_2O_3, and TiN emerge as the most effective ARCs for improving Si solar cell performance.

Keywords: anti-reflective coating, crystalline silicon, heterojunction, PC1D, solar cells

1. INTRODUCTION

A significant challenge for high efficiency silicon heterojunction (SHJ) solar cells is the inherent optical loss from surface reflection, where over 30% of incident sunlight is reflected away by the bare silicon (Si), severely limiting their photo-current and overall performance.[1,2] The anti-reflective coating (ARC) is therefore critical, as it uses destructive interference to cancel out these reflections, dramatically increasing light capture. For high efficiency SHJ solar cells, an optimised, low-temperature ARC is indispensable. This ensures that their advanced electronic architecture translates into superior performance by minimising this primary optical loss and maximising current generation. Essentially, ARCs are thin dielectric layers engineered with a specific thickness and refractive index to exploit destructive interference. Concurrently, this phenomenon cancels out reflected light waves, significantly increasing the amount of incident light coupled into the solar cell. Generally, this directly boosts the photo-generated current and is a fundamental factor for achieving the high efficiencies possible with SHJ technology.

Recent experimental developments in Si(n+)/Si(p) heterojunction solar cells have achieved record-high efficiencies, enhanced operational stability and introduced advanced contact and doping engineering approaches. This, in turn, establishes these devices as promising candidates for next-generation photovoltaic technologies.[3–7] Previous studies recommended applying an optimised ARC with a specifically selected refractive index to the window layer of SHJ solar cells.[8–11] This layer significantly reduces reflectance and increases photo generation on the front surface. ARCs are therefore essential. While multilayer ARCs offer broad spectral suppression, single-layer coating remains attractive for their simplicity, low processing costs and compatibility with SHJ structures. Common single-layer ARC materials, such as silicon dioxide (SiO_2), aluminium oxide (Al_2O_3) and magnesium fluoride (MgF_2), effectively reduce reflectance, though they exhibit narrow anti-reflection bandwidth.[10,12–14] Spin-coated SiO_2 layers, for instance, can lower surface reflectance below 10% and increase power conversion efficiency (PCE) from 11.68%–15.91% by enhancing short-circuit current density (J_{SC}) and open-circuit voltage (V_{OC}).[15] Nevertheless, their minimum reflectance typically occurs at only a single wavelength.[16,17] Similarly, single-layer Al_2O_3 and MgF_2 films improve SHJ performance, with 20 nm Al_2O_3 raising J_{SC} by 1.5 mA/cm^2 and MgF_2 enabling a PCE of 20.8%.[10,18] Still, their reflectance reduction remains wavelength-specific, limiting broadband effectiveness.[19,20]

Despite extensive studies on improving light trapping on Si solar cells, a comprehensive investigation into the interplay between ARC layers on SHJ remains limited.[21–23] Current research often examines these parameters individually, overlooking their combined influence on efficiency.[24–28] Most studies focus on conventional ARC materials, with limited exploration of alternatives such as magnesium oxide (MgO) and titanium nitride (TiN). These may provide unique optical advantages, including low-index interference, high-index plasmonic effects, or combined passivation benefits. In line with this, single-layer ARCs are also constrained by narrow anti-reflection bandwidth and suboptimal performance on textured surfaces under angular illumination.[14,17] Additionally, there is insufficient research on co-optimising optical and electrical properties, such as simultaneously achieving reflectance reduction and effective surface passivation, while ensuring compatibility with low-temperature deposition suitable for SHJ. This work employs PC1D-based optical-electrical simulations to systematically evaluate and compare multiple ARC materials (MgO, Al_2O_3, MgF_2 and TiN) and their spectral responses for SHJ solar cells. Ultimately, this provides a predictive framework to enhance device performance prior to fabrication.

2. METHODOLOGY/SIMULATION

PC1D simulation is a one-dimensional (1D) tool for modelling the electrical and optical behaviour of Si solar cells. It predicts key parameters, including J_{SC}, V_{OC}, fill factor (FF) and PCE. It can simulate single-layer ARCs, surface textures and layer thickness, enabling rapid optimisation before fabrication. Although PC1D is one-dimensional and does not model the actual two-dimensional (2D) or three-dimensional (3D) shape of screen-printed silver contacts, it effectively simulates their core electrical functions. Users define parameters such as contact resistance and surface recombination velocity, allowing the software to replicate how real silver contacts influence series resistance and carrier recombination. Concurrently, this approach enables accurate prediction of the solar cell's electrical performance while simplifying simulation by focusing on critical electrical and optical effects rather than physical geometry. This renders it a powerful tool for optimising Si solar cell design and ARC properties prior to experimental fabrication. Notably, the simulated cell has an area of 110 cm^2, a front reflectance of 10%, a 10 μm window layer and a 100 μm absorber layer composed of n-Si and p-Si in Regions 1 and 2, respectively. Meanwhile, the n-type and p-type background doping levels are set at 1×10^{19} cm^{-3} and 1×10^{16} cm^{-3}, respectively.[29–31] Tables 1 and 2 present the numerical values of the parameters for the Si(n+)/Si(p) HJ. Following this, Figure 1 displays the device schematic using PC1D based on the parameters. Overall, this simulation have been carried out at Solar Energy Research Institute (SERI), Universiti Kebangsaan Malaysia, Universiti Teknologi MARA, Perlis Branch and School of Physics, Universiti Sains Malaysia.

Table 1: Basic solar cell parameters examined using PC1D software

Parameter	Value	
	REGION 1	REGION 2
Thickness (μm)	10	100
Material	Si	Si
Dielectric Constant (eV)	11.9	11.9
Band Gap (eV)	1.124	1.124
Intrinsic Concentration (cm^{-3})		
Type of Background Doping	n-Si	p-Si

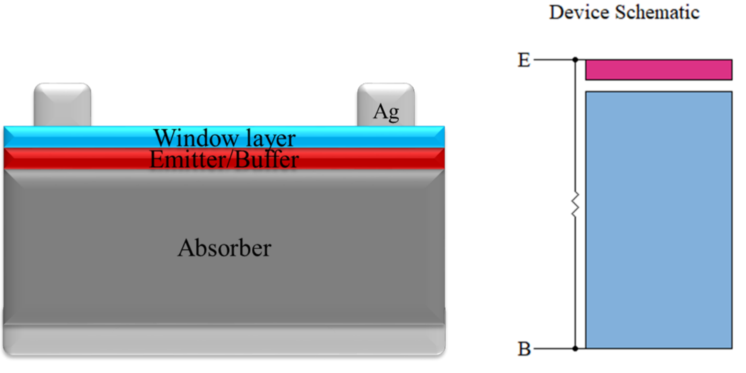
(*continue on next page*)

Table 1: (*continued*)

Parameter	Value	
	REGION 1	REGION 2
Background Doping Concentration (cm^{-3})		
Bulk Recombination (μs)	1000	1000
Excitation Mode		
Excitation Mode	Transient,16 time-steps	
Temperature (⁰C)	25	
Base Circuit (V)	–0.8 to 0.8	
Collector Circuit	Zero	
Constant Intensity (W/cm^2)	0.1	
Spectrum	AM1.5G	

Table 2: Refractive index for ARC on window layer

Anti-reflection (ARC)	Refractive index
SiO_2 [61–64]	1.45
Al_2O_3 [65–67]	1.75
MgF_2 [68,69]	1.38
MgO[70,71]	1.70
TiN[72]	1.29



(a) (b)

Figure 1: Schematic diagram of (a) simple heterojunction and (b) PC1D simulation.

3. RESULTS AND DISCUSSION

Figure 2(a) illustrates that the V_{OC} of a Si solar cell depends strongly on the ARC material and its thickness. Specifically, MgO and Al_2O_3 exhibit the highest V_{OC}, reaching 656 mV and 655.9 mV at 100 nm–110 nm, respectively, as they effectively reduce surface recombination and enhance photon absorption. TiN performs similarly, peaking at 655.8 mV at the same thickness, likely aided by its conductive properties. Nonetheless, its performance decreases slightly by greater thickness due to optical interference. Conversely, MgF_2 and SiO_2 demonstrate lower peak V_{OC}, with MgF_2 reaching 654.7 mV at 130 nm and SiO_2 reaching 653.6 mV at 120 nm–130 nm. While they possess good anti-reflective properties, their passivation is less effective. Despite this, SiO_2 remains widely used in industry for its stability. Overall, high refractive index materials like MgO, Al_2O_3 and TiN enhance light management and V_{OC} more efficiently than low-refractive index options such as MgF_2 and SiO_2.

Figure 2(b) displays the J_{SC} of Si solar cells with different ARC layers. Notably, J_{SC} depends on the ARC's ability to reduce optical losses and enhance photon absorption through its optical properties and thickness. In particular, MgO achieves the highest J_{SC} of 15.39 mA/cm² at 110 nm, thanks to its refractive index ($n \approx 1.72$), which effectively matches air ($n = 1$) to Si ($n \approx 3.4$), minimising reflection. Al_2O_3 follows closely, peaking at 15.31 mA/cm² at 100 nm–110 nm, offering both strong anti-reflection and surface passivation benefits ($n \approx 1.76$). While TiN reaches 15.27 mA/cm² at 100 nm due to its high refractive index ($n \approx 1.78$), it declines at greater thickness due to phase interference. By contrast, MgF_2 ($n \approx 1.38$) and SiO_2 ($n \approx 1.48$) yielded lower J_{SC}, 14.62 mA/cm² and 14.05 mA/cm², respectively, due to higher reflection losses. Thus, high refractive index materials such as MgO, Al_2O_3 and TiN enhance J_{SC} more effectively than low-index options.

According to Figure 2(c), the efficiency of Si solar cells with different ARC layers follows trends similar to those of V_{OC} and J_{SC} in Figures 2(a) and Figure 2(b). MgO, with a refractive index of ~1.72, achieves the highest efficiency of 8.46% at 110 nm and maintains superior performance between 110 and 140 nm, making it the most effective ARC for reducing reflection. Moreover, Al_2O_3 reaches 8.41% at 100 nm–110 nm, offering both high efficiency and surface passivation benefits. TiN also performs well, peaking at 8.39% in the same thickness range. Additionally, MgF_2 ($n \approx 1.38$) recorded its maximum efficiency of 8.02% at 130 nm–140 nm, while SiO_2 ($n \approx 1.48$) reached 7.70% at 120 nm–130 nm, the lowest among the materials studied. Overall, high refractive index ARCs such as MgO, Al_2O_3 and TiN optimise optical interference and light absorption. At the same time, MgO provides the best standalone performance, while Al_2O_3 adds the advantage of surface passivation.

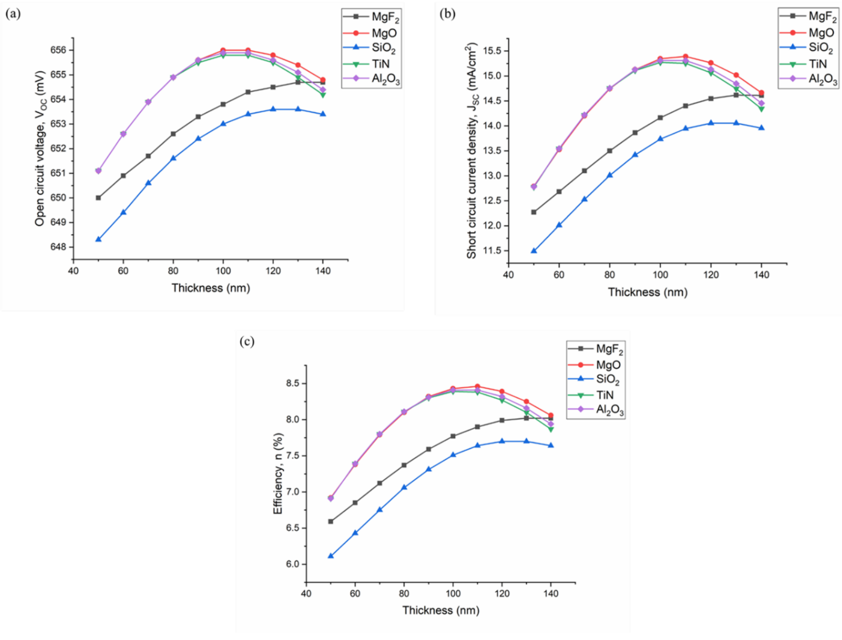


Figure 2: Optimisation of different ARCs layer thickness in terms of (a) $V_{OC,}$ (b) J_{SC} and (c) efficiency.

Figure 3 presents the external quantum efficiency (EQE) of Si solar cells with different ARC layers. Note that Si solar cells without an ARC have the lowest EQE, rising from 26.5% at 300 nm to 56% at 850 nm, then declining beyond 900 nm due to limited photon absorption, high reflection and recombination losses. Adding SiO_2 as an ARC significantly improves EQE, reaching 83.73% at 620 nm, as reduced reflection enhances photon absorption and carrier generation across the visible spectrum. MgF_2 as an ARC further increases performance, with a peak EQE of 86.27% at 640 nm. Compared to SiO_2, MgF_2 reduces reflection losses more effectively, boosting photon absorption and improving overall solar cell efficiency. These results highlight the significance of selecting appropriate ARC materials to maximise EQE and enhance carrier photo generation in Si solar cells.

In addition to that, MgO as an ARC on Si solar cells achieves the highest EQE, peaking at 93.1% at 630 nm and remaining above 90% from 540 nm–750 nm. It outperforms SiO_2 and MgF_2 by reducing reflection losses and enhancing light absorption, which increases carrier generation and overall efficiency. In comparison, TiN reaches a peak EQE of 92.83% at 640 nm, higher than SiO_2 and MgF_2 but slightly lower than MgO, maintaining EQE above 90% from 550 nm–750 nm. TiN also provides stability and durability while improving light absorption. Al_2O_3 achieves a peak EQE of 92.98%

at 640 nm, maintaining above 90% across the same wavelength range and providing surface passivation to reduce recombination losses. Beyond 1,000 nm, all ARC layers presented reduced EQE due to lower photon energy. Overall, Figure 3 confirms that MgO, Al_2O_3 and TiN effectively enhance EQE and solar cell performance compared to traditional ARCs.

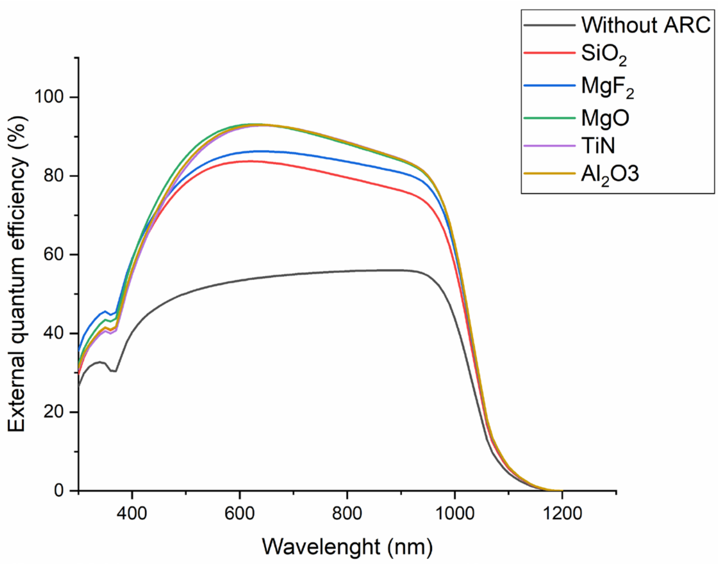


Figure 3: Effects of ARC layers on EQE.

Figure 4 illustrates the total reflectance (TR) of Si solar cells with different ARC layers, including SiO_2, MgF_2, MgO, TiN and Al_2O_3, compared to cells without an ARC (see Figure 8). Cells without an ARC exhibit the highest TR across 300 nm–1,200 nm, reaching 73.49% at 300 nm and stabilising around 42.21% at 1,200 nm, indicating significant optical losses. Adding an ARC significantly reduces TR, enhancing light absorption. Correspondingly, SiO_2 lowers TR to 16% to 18% in the 500 nm–600 nm range, though reflectance increases at longer wavelengths, indicating wavelength-dependent effectiveness. Meanwhile, MgF_2 reduces TR from 64.39% at 300 nm to 13.64% at 640 nm, while MgO achieves a minimum TR of 6.80% at 630 nm, outperforming SiO_2 and MgF_2. Moreover, TiN reaches 7.05% at 650 nm, slightly higher than MgO, and Al_2O_3 decreases TR from 68.66% at 300 nm to 6.91% at 640 nm. Beyond 650 nm, cells without ARC maintain TR above 30%, losing photos in the near-infrared (NIR) range. In general, ARCs create a refractive index gradient that reduces reflection and increases light absorption, thereby improving carrier generation and overall solar cell efficiency.

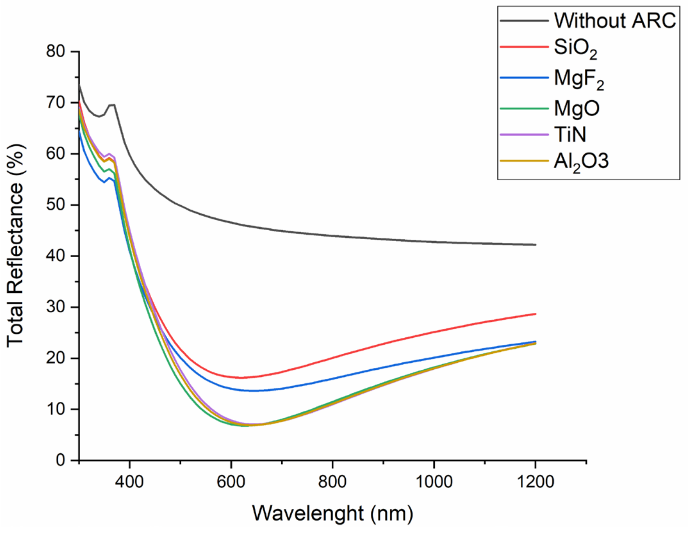


Figure 4: Effects of ARC layers on TR.

In the NIR wavelength range, MgO surpasses Al_2O_3 as an ARC for Si solar cells. While both materials significantly reduce reflectance compared to bare Si, which exceeds 30% between 650 nm and 1,200 nm, MgO consistently exhibits the lowest TR, reaching 6.80% at 630 nm and remaining lower than Al_2O_3 as the wavelength increases. Recent studies using MgO as an ARC on solar cells have demonstrated improved EQE above 600 nm, reduced reflectance effects and enhanced overall efficiency compared to MgF_2, particularly in SHJ devices.[44,45] Other than that, adding Al_2O_3 as an ARC on Si cells performs well, reducing the TR from 45% to a minimum of 6.91% at 640 nm. Al_2O_3, whether used alone or in multilayer coatings, has the potential to reduce surface reflectance, with reported decreases from 44.9% to 29.6% for single-layer coatings and from 9.3% to 4.7% for double-layer coatings across the 300 to 1,100 nm wavelength range.[23,28,46] Taken together, MgO provides more potent suppression of NIR optical losses and more efficient coupling of long-wavelength photons into the Si absorber.

4. CONCLUSION

This study assessed the performance of SiO_2, MgF_2, MgO, TiN and Al_2O_3 single-layer ARCs on SHJ solar cells using 1D PC1D simulation. The results reveal that ARCs significantly reduce front surface reflectance and improve photo generation compared to bare Si, which exhibits the highest reflectance across 300 nm to 1,200 nm, reaching 73.49% at 300 nm and remaining above 42% at 1,200 nm. In particular, MgO achieved the lowest minimum reflectance (6.80% at 630 nm) and the highest EQE performance, reaching 93.1% at 630 nm. TiN and Al_2O_3 also maintained EQE above 90% from 550 nm to 750 nm. Simultaneously, these findings confirm the significance of ARC selection in enhancing J_{SC} and overall efficiency. However, the 1D PC1D model cannot account for real 3D textures, parasitic absorption or deposition variations. In response, future work should explore multilayer ARCs, nano-texturing and micro-texturing and experimental verification to fully validate these simulated improvements and further optimise the optical design of Si solar cells.

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