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Modelling of the Durability of SiO_2 Anti-Reflection Coating on GaAs Solar Cell with Comsol 5.6

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Abstract

This study presents the effect of long-term outdoor exposure on silicon dioxide (SiO_2) antireflection coating (ARC) surface of GaAs solar cell under simulated outdoor conditions. The work was carried out in COMSOL Multi-physics where the effects of principal and Von Mises stress as well as the strain deformation on reflectance, transmittance, and absorption followed by efficiency degradation were analysed. The results indicated that, the Von Mises stress revealed higher stress of $0.013\ GPa$ in the cell with SiO_2 ARC which deform the surface to 14.8% while the cell without coating experience $0.004\ GPa$ and deform the surface to 16.7%. Optical performance after the 40 years exposure showed total reflectance, transmittance, and absorption of 26.5%, 73.2%, and 0.003% for the cell with SiO_2, and 73.5%, 26.4%, and 2.9×10^{-12}% for the cell without ARC respectively. The efficiency of the cell with SiO_2 ARC degraded from 32.9% to 8.7%, while the cell without ARC declined from 19.2% to 2% over the same period. However, the efficiency of the cell with ARC dropped to the initial level of the bare cell after 25 years of outdoor exposure which indicated the lifespan of the SiO_2 ARC at a thickness of 80nm. These outcomes provide valuable insights in coating design that will help to achieved high efficiency and long-lifespan solar cells for deployment in extreme terrestrial climates and space locations.

Keywords: *Antireflection, COMSOL, Durability, GaAs Solar Cell, SiO_2 coatings, Von Mises*

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1. INTRODUCTION

Photovoltaic (PV) technology has emerged as a leading solution to the growing global demand for sustainable and renewable energy. Among the various types of solar cells, Gallium Arsenide (GaAs) based cells have demonstrated superior performance due to their high conversion efficiency and excellent radiation resistance (Leem et al. 2014). However, the long-term performance and structural reliability of these devices heavily depend on the stability of their front surface, particularly under prolonged exposure to extreme environmental conditions such as high temperatures, humidity, wind, and mechanical load (Nalin Venkat et al. 2023).

To minimize reflection losses and enhance light absorption, antireflection coatings (ARCs) such as magnesium fluoride (MgF), titanium dioxide (TiO_2) and silicon dioxide (SiO_2) are commonly applied to the front surface of GaAs solar cells (Ji et al. 2022). These dielectric materials differ significantly in their mechanical, thermal, and optical properties, which can affect not only the initial performance of the device but also its degradation over time. While TiO_2 offers a higher refractive index and better UV resistance, SiO_2 is often preferred for its chemical stability and lower coefficient of thermal expansion (Parajuli et al. 2023).

Several studies have examined the optical performance of ARCs, but less attention has been given to their long-term thermomechanical reliability (Eitner et al. 2011). Prolonged environmental stress, such as continuous exposure to mechanical load, high temperature and relative humidity can induce significant thermal and mechanical stresses within the layered structure (Wohlgemuth and Kempe 2022). These stresses may cause surface deformation, delamination, or even fracture in the coating or at the coating-cell interface, leading to a decline in overall efficiency and mechanical integrity. However, despite the widespread use of ARCs in PV applications, a comprehensive understanding of their long-term behaviour under coupled thermal and mechanical loading remains incomplete (Wohlgemuth and Kempe 2022).

Several efforts have been made by researchers to develop antireflection coatings (ARCs) capable of withstanding harsh abrasion during cleaning and enduring severe environmental conditions. Nishioka et al., (2019) evaluated the effectiveness of antireflective and anti-soiling, as well as the long-term reliability, of a silica-based coating applied to $Cu(In, Ga)Se_2$ photovoltaic (PV) modules over a five-year period. The results showed that the coating remained effective without significant degradation after 3.5 years. Similarly, Karas et al., (2020) fabricated crystalline silicon solar cells with copper-plated, tin and nickel front contacts and subjected them to extended damp heat conditions (85°C and 85% relative humidity). The results indicated degradation affecting both the series resistance and diode quality, suggesting deterioration of the p-n junction. Owen-Bellini et al., (2021) applied a two-phase testing protocol to assess the performance of crystalline silicon under prolonged high humidity and temperature, simulating a harsh tropical climate. After 120 days, micro-crack failures were observed in the solar cells. Ekinci et al., (2022) investigated the abrasion resistance of ARCs by subjecting them to regular cleaning cycles using different abraders. No visible damage was noted under 1 N and 2 N loads with a felt pad, but significant scratching occurred when Cs-10 and Cs-8 abraders were used. Zeng et al., (2023) analysed silica (SiO_2) ARCs from various manufacturers based on their optical properties, abrasion resistance, and outdoor reliability. The study found a reduction in optical performance in dense coatings; however, these coatings offered superior durability and extended service life. Despite these advancements, the effect of long-term outdoor exposure on mechanical and optical properties of SiO_2 ARCs remain largely unexplored.

In this work, the effects of prolong outdoor exposure on GaAs solar cell surface with and without $\mathrm{SiO_2}$ ARC were evaluated using COMSOL Multi-physics software. The Principal stress, von Mises stress, and deformation distribution and their effects on optical and electrical properties were analysed within the simulated period of 40 years. The results will provide a foundation for material selection in long-lifespan solar system and contribute to the design of more reliable PV technologies.

2. MATERIALS AND METHOD

The materials used in this work include COMSOL Multi-physics software version 5.6 and its virtual silicon dioxide as anti-reflection coating while gallium arsenide solar cell as a substrate. The simulated structure of the solar cell was made up of two layers for cell without ARC and three layers for solar cell with coating (n-type GaAs, p-type GaAs and ARC) in a stratified arrangement.

The geometrical two-dimensional structure was selected based on previous literature (Abu-Shamleh et al., (2021), Parajuli et al., (2023)). As shown in Figure 1, the dimension of the $GaAs$ solar cell (n and p) and antireflection coating was set to 600nm by 100nm and 80nm by 100nm in height and width respectively.

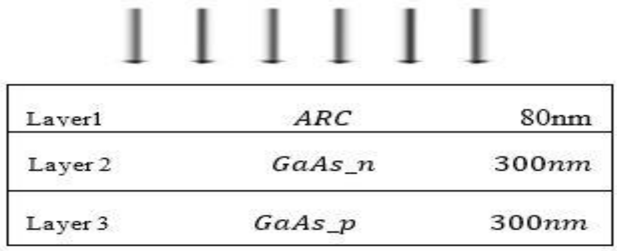


Figure 1: *The diagram of GaAs solar cell coated with ARC (Parajuli et al., 2023)*

This structure was created in COMSOL build in environment. Most of the material properties shown in Table 1 were sourced from COMSOL Library while others from relevant literature (Eitner *et al.*, (2011), Parajuli *et al.*, (2023)). The materials properties were then inserted in the respective layers (cell and coatings) (Hägglund and Gauthier 2019).

Table 1: *Material properties of GaAs solar cell (n and p-type) and SiO_2 ARC*

Input Parameters	$\boldsymbol{GaAs\ (n)}$	$\boldsymbol{GaAs\ (p)}$	**SiO_2 ARC**
Relative permittivity	13.8	13.8	2.13
Band gap	$1.4V$	$1.4V$	9.0V
Refractive Index	3.6	3.6	1.46
Electron affinity	$4.2V$	$4.2V$	-
Effective density of state (Nc)	$1 \times 10^{16} cm^{-3}$	$3 \times 10^{18} cm^{-3}$	-
Effective density of state (Nv)	$1 \times 10^{16} cm^{-3}$	$3 \times 10^{18} cm^{-3}$	-
Electron mobility	$500 cm^2/Vs$	$500 cm^2/Vs$	-
Hole mobility	$300 cm^2/Vs$	$300 cm^2/Vs$	-
Electron lifetime	$100 \mu s$	$100 \mu s$	-
Hole lifetime	$100 \mu s$	$100 \mu s$	-
Temperature	$300K$	$300K$	300K
Donor concentration	$9 \times 10^{19} cm^{-3}$	$1 \times 10^{21} cm^{-3}$	-
Power intensity	$0.1 W/cm^2$	$0.1 W/cm^2$	$-$
Applied Voltage	1.3V	1.3V	-
Young Modulus	85GPa	85GPa	72GPa
Thermal conductivity	$46 Wm^{-1}K^{-1}$	$46 Wm^{-1}K^{-1}$	$1.4 Wm^{-1}K^{-1}$

Density	$5500 Kgm^{-3}$	$5500 Kgm^{-3}$	$2200 Kgm^{-3}$
Specific heat capacity	$330 JKg^{-1}K^{-1}$	$330 JKg^{-1}K^{-1}$	$703 JKg^{-1}K^{-1}$
Coefficient of thermal expansion	$5.8 \times 10^{-6} K^{-1}$	$5.8 \times 10^{-6} K^{-1}$	$0.55 \times 10^{-6} K^{-1}$
Poisson ration	0.31	0.31	0.17

During the simulation, boundary conditions of electromagnetic wave, semiconductor and heat transfer in solid as well as the structural mechanic modules were appropriately defined so as to mimic the real-life scenarios.

The temperature distribution of GaAs solar cell with and without SiO_2 ARC was analyse using different boundary condition of heat transfer in solid modules which include surface-to-ambient radiation, convective heat flux, and boundary heat source. For stresses response (minimum, intermediate, maximum, and Von Mises) and deformation evaluation, the coated cell were exposed to the simulated period of 40 years under extreme outdoor condition (500K, 85% relative humidity, and wind speed of $5ms^{-1}$) (Owen-Bellini et al. 2021)(Bharatish et al. 2015). The outdoor condition was simulated by coupling the electromagnetic wave and heat transfer in solid module. Moreover, the effects of stresses and deformation on optical and electrical properties of the cell with and without ARC were investigated using electromagnetic wave, semiconductor and structural mechanics modules. The simulation study was then computed using time-dependent. Lastly, the efficiency degradation from all the coated and uncoated solar cell was calculated and plotted from the simulation results.

3. RESULT AND DISCUSSION

The front surface of GaAs solar cell coated with and without SiO_2 ARC were exposed to the simulated outdoor conditions for a period of 40-years. In this period, the effects of Principal and Von Mises stresses and surface deformation on optical and electrical properties were investigated.

3.1 Principal Stress Distribution on GaAs Solar Cell with and without SiO_2 ARC

When the cell with ARC exposed to outdoor condition of temperature 500K, 85% relative humidity and $5ms^{-1}$ wind speed, it experience different stresses including principal and Von Mises stress.

Principal stress refers to the maximum to minimum normal stresses that act perpendicular to the surface of the material or at a given point. Figure 3a-3c presents the first, second and third principal stress as the maximum, intermediate and minimum stress respectively while Figure 3d presents Von Mises stress.

Figure 3a presents the distribution of the third principal stress as the minimum stress experience by the solar cells with and without ARC after 10 years of exposure.

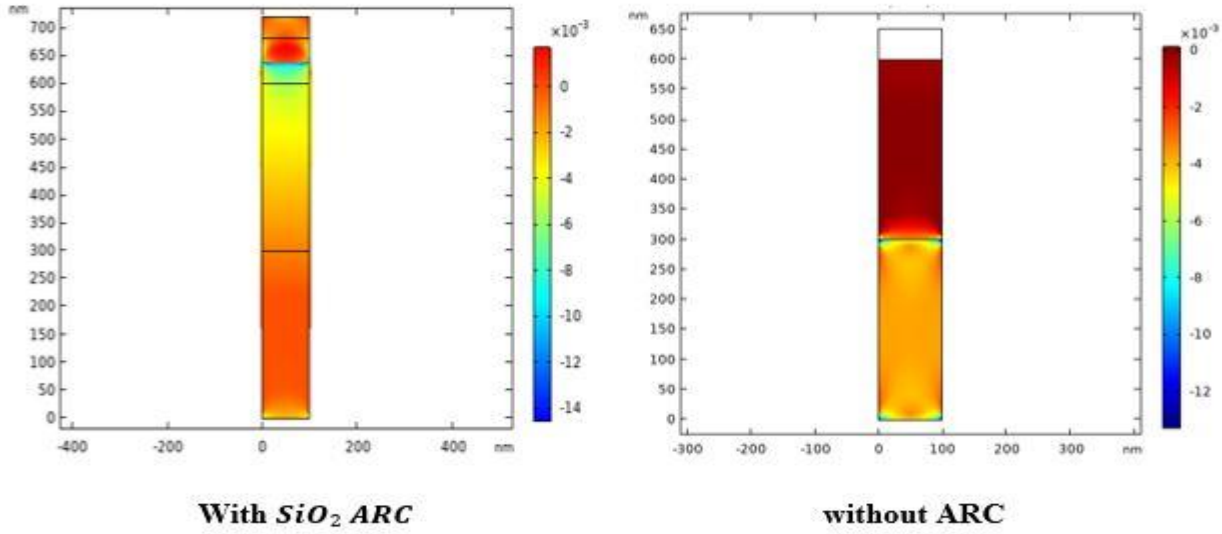


Figure 3a: *Distribution of third principal stress (GPa) on GaAs solar cells with and without SiO_2 ARC*

As shown in the figure, the GaAs solar cell with the SiO_2 coating displays higher stress (indicated by red) and distributed across the cell, especially at the coating surface. However, the n-layer of solar cell without ARC experience higher stress concentration compared to the one with coating.

Figure 3b presents the distribution of second principal stress as the intermediate stress experience by the solar cell with and without ARC under 25 years of exposure.

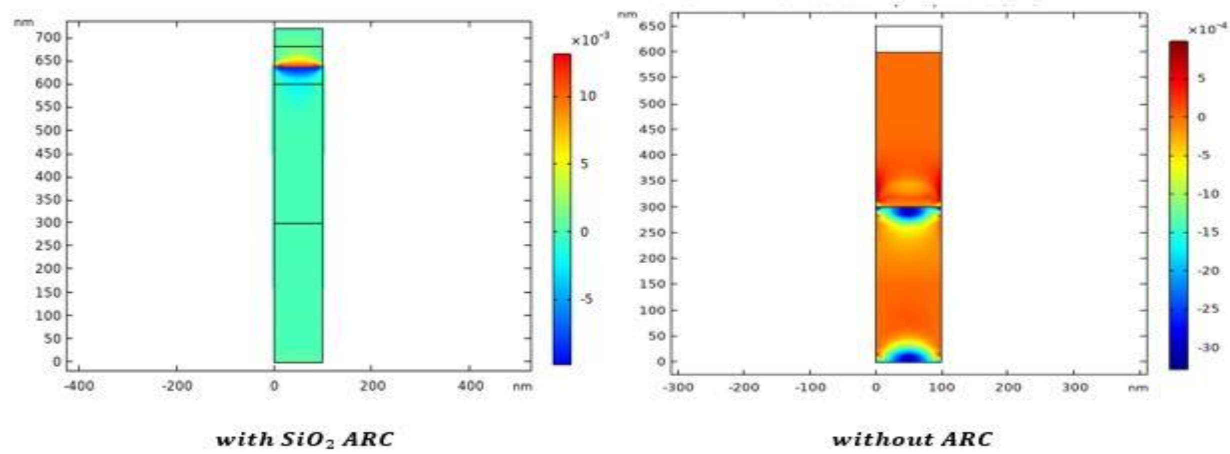


Figure 3b: *Distribution of the second principal stress (GPa) of GaAs solar cell with and without SiO_2 ARC*

The high stress magnitude of $0.010GPa$ concentrated at cell-coating interface in cell with ARC. Due to the coefficient of thermal expansion mismatch between the coating and the cell, the stress was directed upward toward the coating surface. This enhance the thermal stability and good adhesion at the cell-coating interface, since it experience less stress. However, the SiO_2 coating's surface is more prone to crack and deformation over time due to the direction of the stress, which could adversely affect its optical properties. Although, the lower stress in the solar cell without coating was distributed across the cells but it concentration at n-layer can distort the p-n junction or degrade the electrical properties of the cell.

Furthermore, Figure 3c presents the distribution of the first principal stress, as the maximum stress, with a magnitude of 14×10^{-3} GPa for solar cell with SiO_2 ARC and 0.7×10^{-3} GPa for solar cell without ARC.

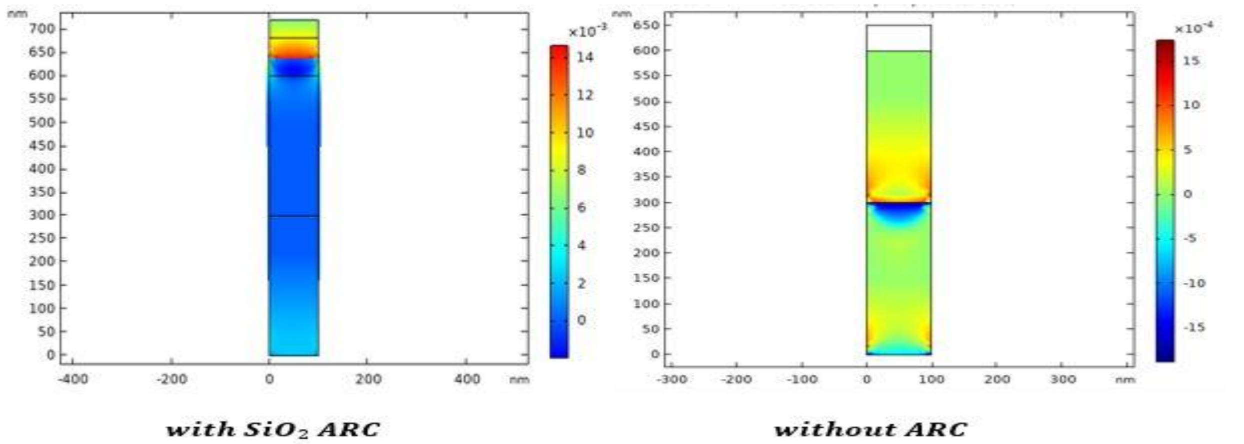


Figure 3c: *Distribution of the First Principal stress (GPa) of GaAs solar cell with and without SiO_2 ARC*

As shown in the figure, the stress in the cell with SiO_2 ARC is directed upwards and concentrated at the coating surface. This behaviour led to the compressive stress and rapid coating surface deformation. This will change the coating surface structure which negatively affects the optical performance by obstructing photon absorption. In contrast, the solar cell without coating, maintain its stress status but with high magnitude at n-layer.

Figure 3d presents the Von Mises stress as the stress tensor that use to predict whether the solar cells with and without ARC will yield or fail under long-term exposure.

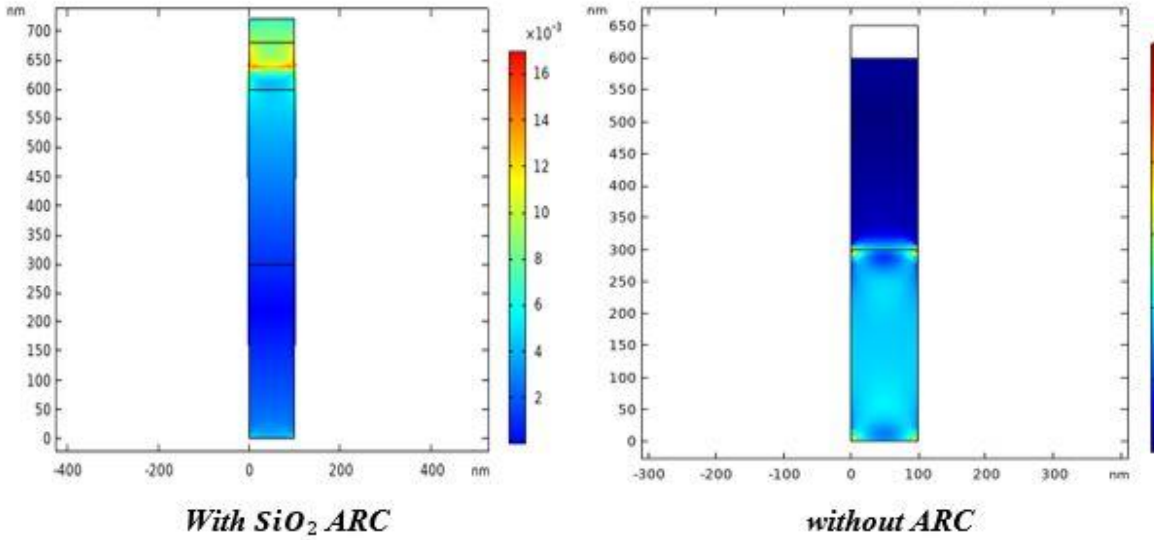


Figure 3d: *Distribution of the Von Mises stress (GPa) of GaAs solar cell with and without SiO_2 ARC*

As seen from the figure, the cell with SiO_2 ARC has the larger magnitude of Von Mises stress of 0.013GPa. However, the stress is distributed laterally within the coating especially at cell-coating interface. This demonstrates that, the coating layer will face much more deformation than the rest of the solar cell. Due to the initial direction of the stress at the cell without ARC, the cell has a low stress of 0.005GPa which is concentrated at the p-layer. Despite the lower stress magnitude in the cell without ARC, the n and p layer will be degraded more compared to the coated cell.

Furthermore, comparing the fracture strength of the coated cell with its Von Mises stress indicated that, the magnitude of the Von Mises stress of SiO_2 ARC ($0.013\ GPa$) exceeds its fracture strength of $8MPa$ at 80nm thickness. This leads a compressive stress that causes the coating deformation.

3.2 Deformation of $GaAS$ Solar Cell with and without SiO_2 ARC

Deformation can be either constrained or unconstrained (free stress), depending on the nature of the stress applied. Over time, as the coating is subjected to long-term exposure, its structure can bend, crack, and delaminate as shown in Figure 4.

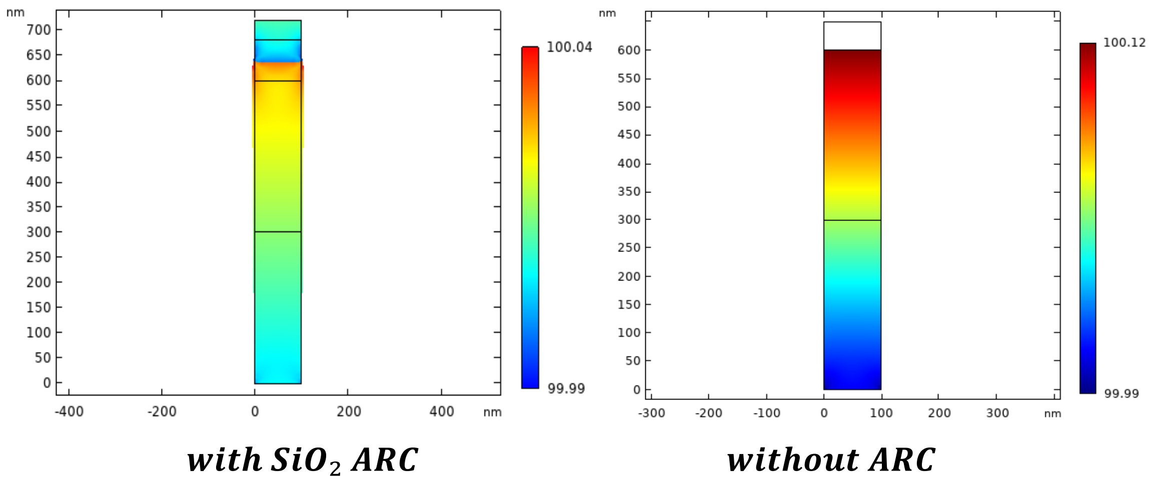


Figure 4: *Structural Deformation of GaAs solar cell coated with and without SiO_2 ARC*

From the figure, it is evident that the SiO_2 coating deforms with a strain (increase in length per original length) deformation of 14.8%, primarily from the surface to the cell-coating interface protecting the solar cell from much deformation. In contrast, the solar cell without ARC deforms significantly with strain deformation of 16.7%, extending to the p-n junction form the cell surface. The high deformation causes the cell and coating surface structure to shrink and delaminate and the structural changes of the coating due to deformation can impact the optical properties.

3.3 Effect of stress on optical properties of GaAs Solar cell with and without SiO_2 ARC

The optical properties of the coating materials play a crucial role in enhancing the efficiency of solar cells. However, the structural changes in the coating due to prolong stress can affect the reflectance, transmittance, and absorption, as shown in Figures 5a-c.

Figure 5a presents the effect of stress on total reflectance of the cell with and without SiO_2 ARC.

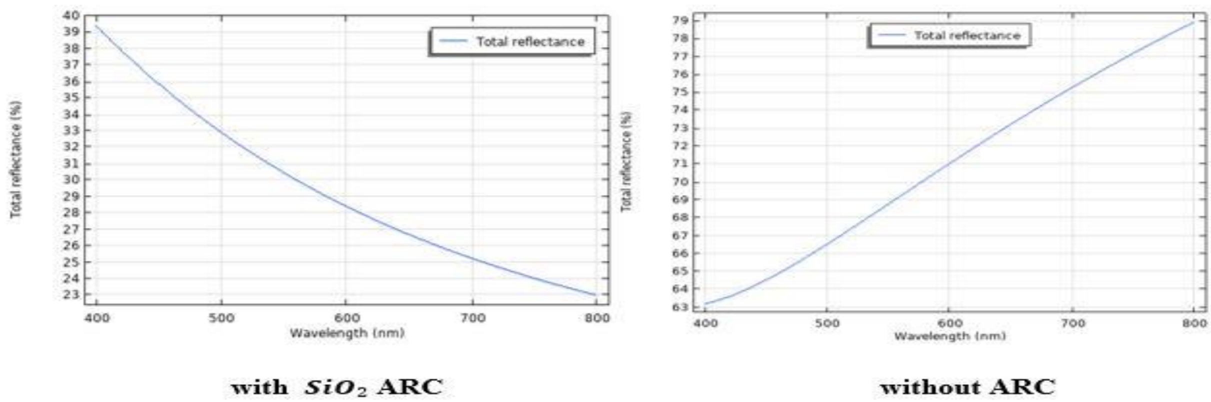


Figure 5a: *Effect of stress on total reflectance of GaAs solar cell with and without SiO_2 ARC*

The total percentage reflectance of the solar cells with and without ARC increases for both the materials, as depicted in Figure 5a. The percentage reflectance of the solar cell with and without ARC at 650nm was found to be 26.5 and 73% respectively. This increase is attributed as a result of prolong stress which cause the change in surface structure due to deformation of the coatings and solar cell where it affects optical parameters such as the refractive index.

Figure 5b illustrates the total transmittance of the solar cell with and without ARC, since according to Fresnel, reflectance is inversely related to transmittance.

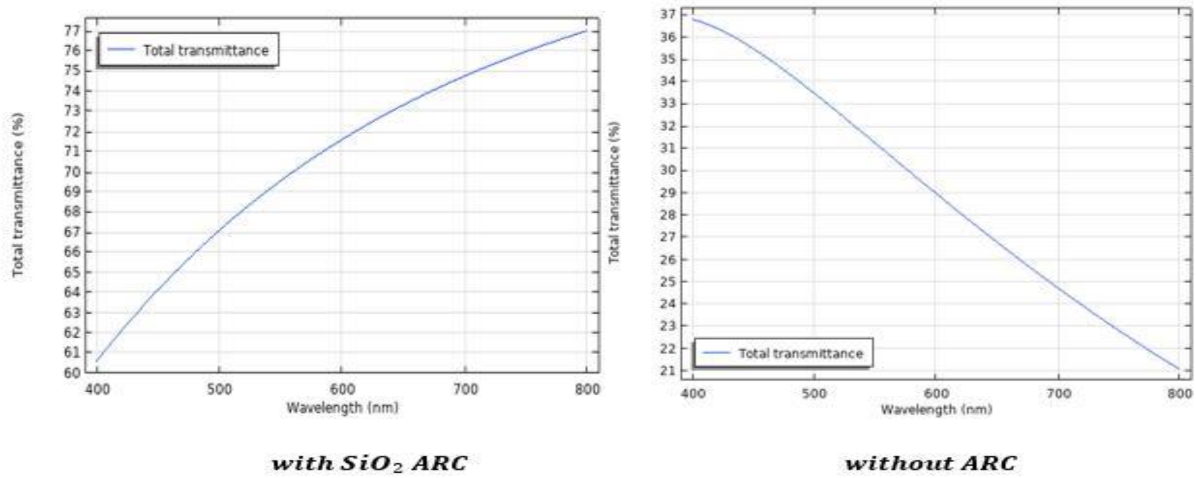
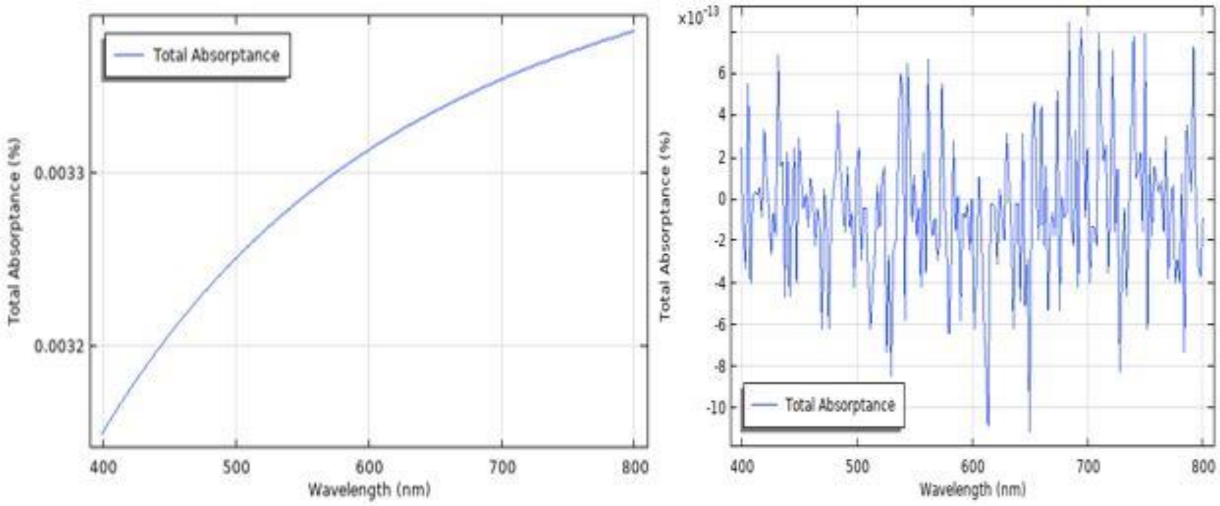


Figure 5b: *Effect of stress on total transmittence of GaAs solar cell coated with and without SiO2 ARC*

As observed from the figure, the total transmittance of the solar cell with SiO_2 ARC show high transmittance. This confirms the naturally high transmittance of the SiO_2 ARC, as it is highly transparent. The total percentage transmittance for the solar cells with and without SiO_2 coating were found to be 73.2% and 26.4%, respectively, at a wavelength of 650 nm. The wide difference was arose as a result of the cell surface deformation that altered the refractive index and increased the reflection unlike the coating surface which able to prevents the refractive index alteration.

Even though, high transmission does not necessarily lead to high absorption (since photon absorption is influenced by the solar cell's energy band gap), as illustrated in Figure 5c, especially in the case of cell coated with SiO_2 ARC.



With SiO_2 ARC **Without ARC**

Figure 5c: *Effect of stress on total absorption of GaAs solar cell with and without SiO_2 ARC*

As shown in Figure 5c, the total absorption of the solar cell with and without ARC decreases significantly compared to their normal conditions. At 650 nm, the total absorption of the solar cells with and without SiO_2 ARCs was found to be 0.0033%, and 2.9×10^{-12}% respectively. The low absorption identified at the cell without ARC was due to photon abstraction at the surface of the cell.

The reduction in transmittance and absorption, along with the increase in reflectance, negatively affects the electrical properties of the solar cells with and without ARC, including short-circuit current density, open-circuit voltage, maximum power output, and overall efficiency.

3.4 Effect of stress on electrical properties of GaAs Solar Cell with and without SiO_2 ARC

Figures 6a and 6b illustrate the electron and hole concentrations in GaAs solar cells with and without SiO_2 anti-reflection coatings after 40 years of exposure. The stress-induced defects arising from long-term exposure significantly affect the concentration of electrons and holes at n-type and p-type layer respectively.

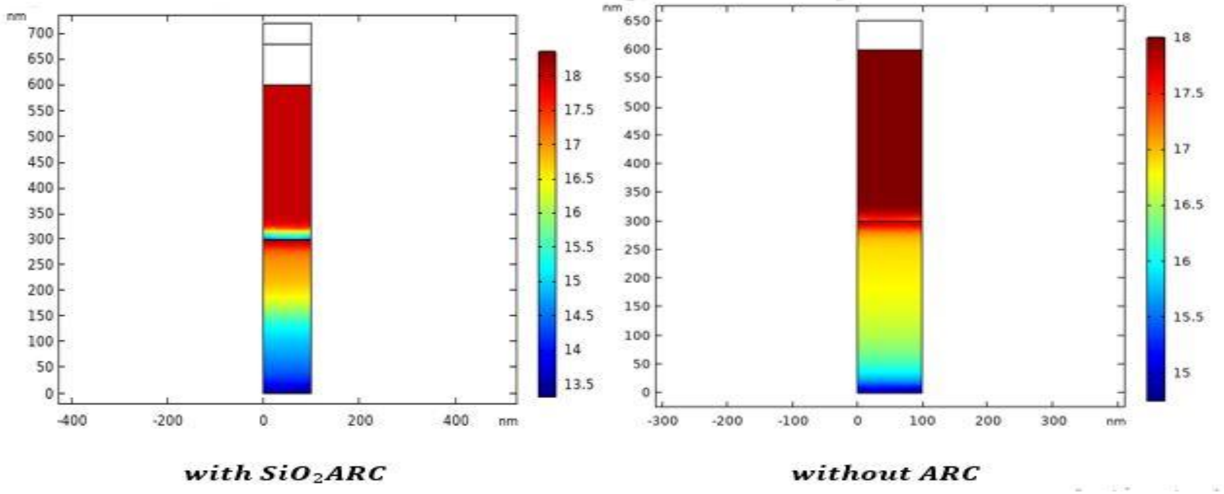


Figure 6a: *Effect of stress on electron contration of GaAs solar cell with and without* SiO_2

Looking at Figure 6a, the cell with SiO_2 ARC has the lower electron concentration especially at the p-n junction. This was attributed due to the formation of interstitial defects at the p-n junction during the deformation of the cell. These defects act as recombination centres (traps) that capture free electrons and shorten carrier lifetimes which in turn degrades both the open-circuit voltage and short-circuit current as also clearly found in the work of Karas et al., (2020). In contrast, the electron concentration of the solar cell without coating is high which revealed the presence of few defects within the cell.

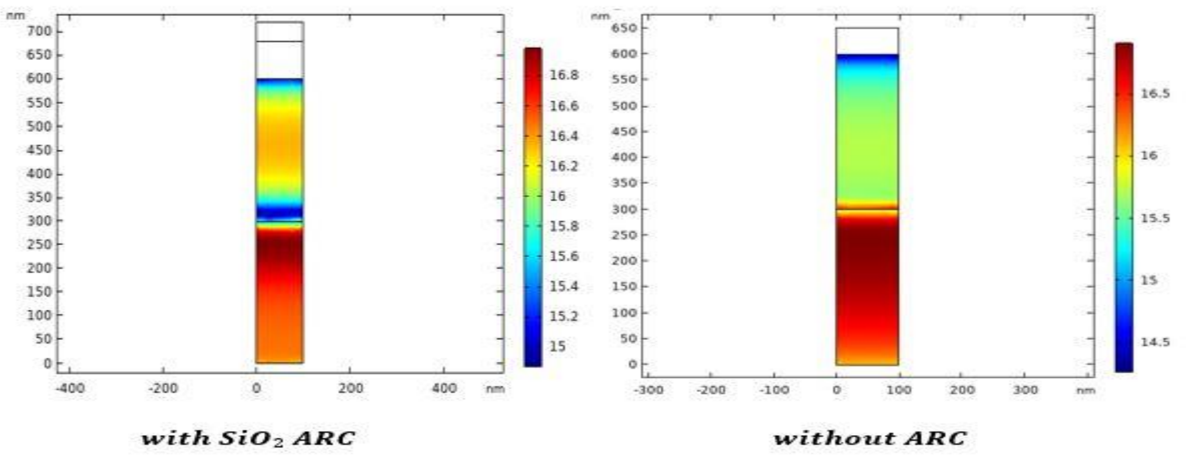


Figure 6b: *Effect of stress on hole concentration in GaAs solar cell with and without* SiO_2 *ARC*

Figure 6b show that, the hole concentration in the cell without coating is lower than that of the SiO_2 coated cell. This occurred due to the formation of the stress hotspot at p-layer. Over time, the effective carrier concentration (for both n-type and p-type carriers) decreases in stressed regions because the traps capture electrons and holes before they contribute to the current generation. High-stress regions, particularly in the GaAs solar cell p-n junction demonstrate the predominance of recombination that intensifies over time, as reflected in Figure 3c. Furthermore, extreme stress can distort the p-n junction, alter the electric field, change the built-in potential, and degrade the junction quality, all of which hinder carrier separation at the depletion layer.

Figure 7 present the efficiency degradation of the coated cell with and without SiO_2 ARC which arose as a result of the prolong stress.

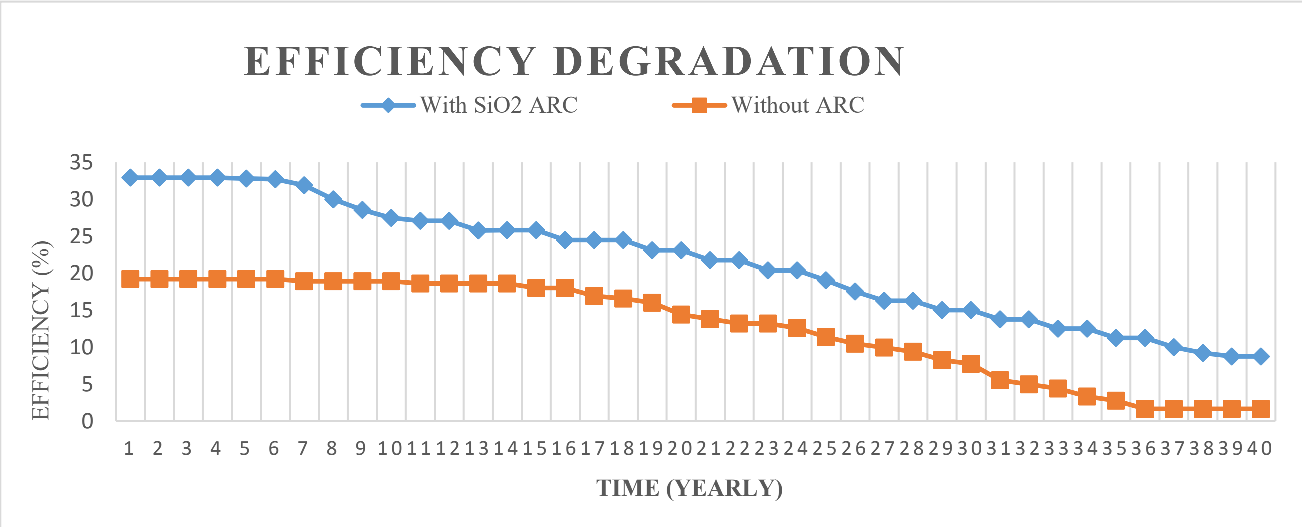


Figure 7: *Efficiency degradation of GaAs solar cell with and without SiO_2 ARC*

When the solar cell exposed to long term outdoor exposure, it optical and electrical properties experience much deterioration as shown in the previous results. Therefore the solar cell efficiency most also degraded overtime. However, despite the deformation experienced by both the solar cell surface, they were able to sustain their initial efficiency of 32.9% and 19.2% for about six (6) years for cell with and without ARC respectively. It later gradually declines to the end level of 8.7% and 2% respectively. However, after 25 years the efficiency of the coated cell was dropped to initial efficiency of the cell without coating which indicated the lifespan of SiO_2 ARC.

Table 2 presents a general comparison of the effects of stress on GaAs solar cells with and without SiO_2 ARCs under long term extreme outdoor conditions.

Table 2: General comparison of stress effect between GaAs solar cell with and without SiO2 ARC

Parameters	*without ARC*	*with SiO_2 ARC*
Magnitude of First principal stress (GPa)	0.7×10^{-3}	14×10^{-3}
Magnitude of Second principal stress (GPa)	0.4×10^{-3}	0.001
Magnitude of Third principal stress (GPa)	2×10^{-4}	0.002
Magnitude of Von Mises stress (GPa)	5×10^{-3}	0.013
Deformation (%)	14.8	16.7
Total reflectance (%)	73.5	26.5
Total transmittance (%)	26.4	73.2
Total absorption (%)	2.9×10^{-12}	0.003
Initial Efficiency (%)	19.2	32.9
Efficiency after 40 years (%)	2	8.7

The results were validated with the practical work of Noman et al., (2022), where the reliability analysis on photovoltaic modules from 35 years PV installation site in Pakistan was carried out. The results found that, the efficiency of the poly crystalline (solar flash) silicon solar module without coating was reduced from the initial value of 10.48% to 2.9% before 30 years of field exposure. Also the work of Nishioka et al., (2019) correspond to this work in term of initial efficiency degradation where the coated cell at 120nm maintain the initial efficiency for 3.5 years.

4. CONCLUSION

We found that, SiO_2 as an ARC on GaAs solar cell under simulated outdoor environmental exposure remain beneficial in enhancing the efficiency of solar cell to span up to 25 years based on the efficiency degradation, stress effects and deformation distribution. The efficiency of GaAs solar cells with and without SiO_2 degraded within the simulated period from 32.9% to 8.7% and 19.2% to 2% respectively. The Von Mises stress of 0.013GPa and 0.005GPa experienced by the solar cell with and without SiO_2 ARC impact both the solar cell to display strain deformation of 14.8% and 16.7% respectively. However, the optical evaluation revealed the effects of these stresses and deformation on the solar cell surface with and without ARC where the percentage total reflectance, transmittance and absorption were obtained as 26.5%, 73.2%, and 0.003 for SiO_2 surface and 73.5%, 26.4% and 2.9×10^{-12}% for cell surface. These results indicated that despite the significant stress effects that change the surface structure and distort the electrical properties of the SiO_2 ARC, it possesses the optical and mechanical advantage to withstand long-term exposure to the solar cell system operating conditions. However, based on the results obtained, this work recommends that while SiO_2 may enhance solar cell performance, its optical and thermal properties must be carefully considered. Therefore, improved ARC design must balance mechanical durability, thermal behaviour, and optical properties to ensure the long-term viability of solar cells in extreme terrestrial and space environments.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

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